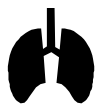# Chapter 5
Estimation of Media Concentrations

What's Covered in Chapter 5:

◆　　　Calculation of COPC Concentrations in Air for Direct Inhalation

◆　　　Calculation of COPC Concentrations in Soil

◆　　　Calculation of COPC Concentrations in Produce

◆　　　Calculation of COPC Concentrations in Beef and Dairy Products

◆　　　Calculation of COPC Concentrations in Pork

◆　　　Calculation of COPC Concentrations in Chicken and Eggs

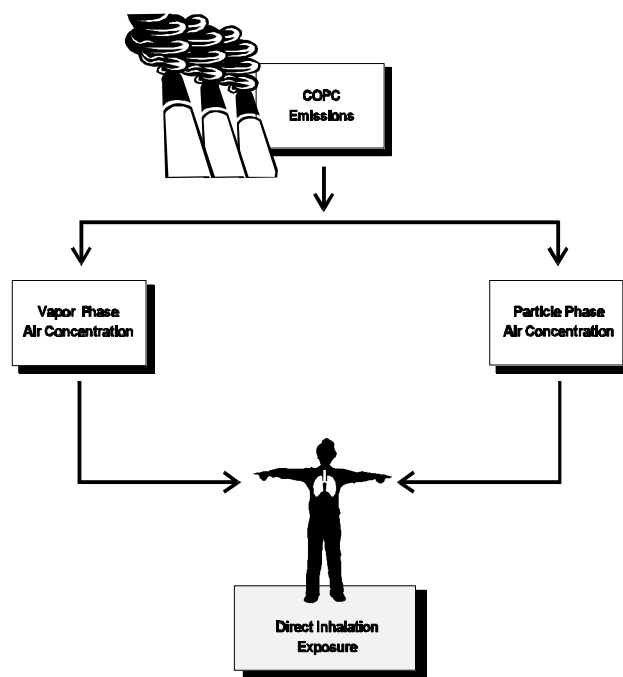◆　　　Calculation of COPC Concentrations in Drinking Water and Fish

The purpose of this chapter is to describe the estimating media concentration equations and associated parameters used in evaluation of the recommended exposure scenarios presented in Chapter 4. The origin and development of each of these equations, and description of associated parameters, are presented in most cases. The equations are also presented in Appendix B without derivation, and organized according to exposure pathway. Discussions of ISCST3 modeled unitized air parameters and compound specific parameters required in the estimating media concentration equations are presented in Chapter 3 and Appendix A-3, respectively. Appendix A-3 also provides recommended values for the compound specific parameters. Equations for use in modeling phase allocation and speciation of mercury concentrations are presented and discussed in Appendix B. Also, it should be noted that reference made throughout Chapter 5 to particle phase is generic and made without distinction between particle and particle-bound.

Section 5.1 describes the estimating media concentration equations used to support evaluation of direct inhalation of COPCs. Section 5.2 describes the estimating media concentration equations for soils contaminated by COPCs. Section 5.3 describes the estimating media concentration equations used to determine COPC concentrations in produce. Sections 5.4 through 5.6 describe equations used to determine COPC concentrations in animal product (such as milk, beef, pork, poultry, and eggs) resulting from animal ingestion of contaminated feed and soil. Section 5.7 describes equations used to determine COPC concentrations in fish through bioaccumulation (or, for some compounds, bioconcentration) from the water column, dissolved water concentration, or bed sediment—depending on the COPC.

5.1   CALCULATION OF COPC CONCENTRATIONS IN AIR FOR DIRECT INHALATION

COPC concentrations in air are calculated by summing the vapor phase and particle phase air concentrations of COPCs. Air concentrations used in the evaluation of long-term or chronic exposure, via direct inhalation, should be calculated using unitized yearly air parameter values as specified in Appendix B, Table B-5-1. Air concentrations used in the evaluation of short-term or acute exposure, via direct inhalation, should be calculated using unitized hourly air parameter values as specified in Appendix B, Table B-6-1.


Figure 5-1 - COPC Concentration in Air for Direct
Inhalation

5.2   CALCULATION OF COPC CONCENTRATIONS IN SOIL

COPC concentrations in soil are calculated by summing the vapor phase and particle phase deposition of COPCs to the soil. Wet and dry deposition of particles and vapors are considered, with dry deposition of vapors calculated from the vapor air concentration and the dry deposition velocity. The calculation of soil concentration incorporates a term that accounts for loss of COPCs by several mechanisms, including leaching, erosion, runoff, degradation (biotic and abiotic), and volatilization. These loss mechanisms all lower the soil concentration associated with the deposition rate. Equations for

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the calculation of soil concentration and soil losses of COPCs are presented in Appendix B, Tables B-1

for land use areas, and Tables B-4 for watersheds (see Section 5.7).
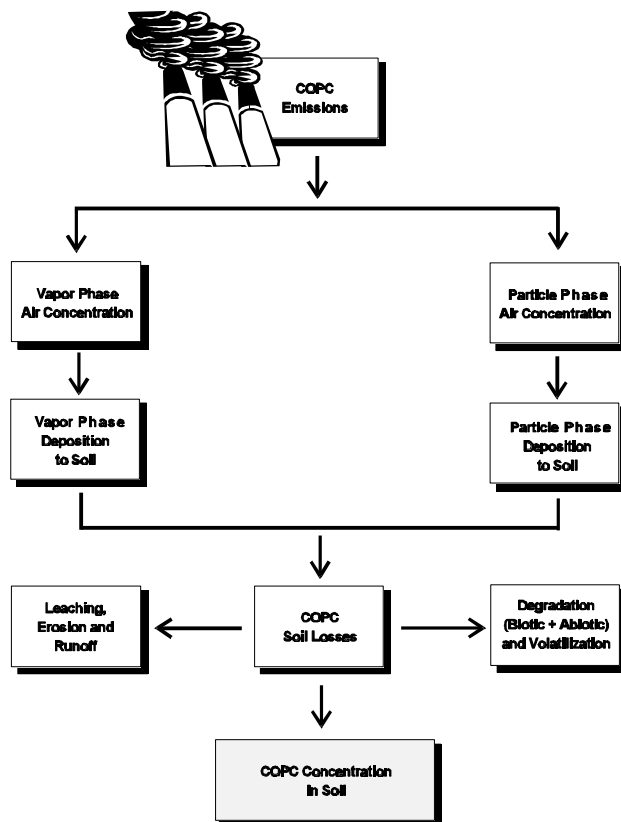
Figure 5-2 - COPC Concentration in Soil

Soil concentrations may require many years to reach steady state. As a result, the equations used to

calculate the average soil concentration over the period of deposition were derived by integrating the

instantaneous soil concentration equation over the period of deposition. For carcinogenic COPCs,

U.S. EPA OSW recommends using two variations of the equation (average soil concentration over

exposure duration):

(1)   one variation to be used if the exposure duration is greater than or equal to the operating
        lifetime of the emission source or time period of combustion, and

(2)   the other form to be used if the exposure duration is less than the operating lifetime of
        the emission source or time period of combustion.

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For noncarcinogenic COPCs, U.S. EPA OSW recommends using the second form of the carcinogenic equation to calculate the highest 1-year annual average soil concentration; typically occurring at the end of the operating lifetime of the emission source. These equations are described in more detail in Section 5.2.1.

Soil conditions—such as pH, structure, organic matter content, and moisture content—affect the distribution and mobility of COPCs. Loss of COPCs from the soil is modeled by using rates that depend on the physical and chemical characteristics of the soil. These variables and their use are described in the following subsections, along with the recommended equations.

5.2.1   Calculating Cumulative Soil Concentration (*Cs*)

U.S. EPA (1990e) recommended the use of the following equation—adapted from Travis, Baes, and Barnthouse (1983)—to calculate cumulative soil concentration:

$$Cs = \frac{100 \cdot (Dydp + Dywv) \cdot [1.0 - \exp (-ks \cdot tD)]}{Z_s \cdot BD \cdot ks}$$ Equation 5-1

where

Cs	=	Average soil concentration over exposure duration (mg COPC/kg soil)
Dydp	=	Unitized yearly dry deposition from particle phase (s/m^2-yr)
Dywv	=	Unitized yearly wet deposition from vapor phase (s/m^2-yr)
ks	=	COPC soil loss constant due to all processes (yr^{-1})
tD	=	Time period over which deposition occurs (time period of combustion) (yr)
100	=	Units conversion factor (mg-m^2/kg-cm^2)
Z$_s$	=	Soil mixing zone depth (cm)
BD	=	Soil bulk density (g soil/cm^3 soil)

U.S. EPA (1993h) stated that this equation evaluated deposition of particle phase COPCs, but fails to

$$Cs = \frac{100 \cdot (Dydp + Dywv + L_{dif}) \cdot [1.0 - \exp (-ks \cdot tD)]}{Z_s \cdot BD \cdot ks}$$ Equation 5-1A

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consider vapor phase deposition or diffusion. To account for vapor phase diffusion, U.S. EPA (1993h)

recommended using the following equation:

where

Cs	=	Average soil concentration over exposure duration (mg COPC/kg soil)
100	=	Units conversion factor (mg-m^2/kg-cm^2)
$Dydp$	=	Unitized yearly dry deposition from particle phase (s/m^2-yr)
$Dywv$	=	Unitized yearly wet deposition from vapor phase (s/m^2-yr)
L_{dif}	=	Dry vapor phase diffusion load to soil (g/m^2-yr)
ks	=	COPC soil loss constant due to all processes (yr^{-1})
tD	=	Time period over which deposition occurs (time period of combustion) (yr)
Z_s	=	Soil mixing zone depth (cm)
BD	=	Soil bulk density (g soil/cm^3 soil)

However, subsequent U.S. EPA guidance (1994g) recommended the use of the original Equation 5-1,

recommended by U.S. EPA (1990e), but limited its use to calculating cumulative soil concentration (*Cs*)

for 2,3,7,8-TCDD only. The discussion stated that the COPC soil loss constant (*ks*) is equal to 0 for all

other COPCs (U.S. EPA 1994g). For COPCs other than 2,3,7,8-TCDD, the following equation—which

eliminates the COPC soil loss constant—was recommended by U.S. EPA (1994g):

$$Cs \ = \ 100 \cdot \frac{Dydw + Dyww}{Z_s \cdot BD} \cdot tD$$

<div align="right">Equation 5-1B</div>

where

Cs	=	Average soil concentration over exposure duration (mg COPC/kg soil)
100	=	Units conversion factor (mg-m^2/kg-cm^2)
$Dydw$	=	Dyd (s/m^2-yr)
$Dyww$	=	Dyw (s/m^2-yr)
tD	=	Time period over which deposition occurs (time period of combustion) (yr)
Z_s	=	Soil mixing zone depth (cm)
BD	=	Soil bulk density (g soil/cm^3 soil)

More recent guidance documents—U.S. EPA (1994r) and NC DEHNR (1997)—recommended two

different equations (Equations 5-1C and 5-1D) for use with carcinogenic COPCs. Equation 5-1C was

recommended for $T_2 \le tD$ and Equation 5-1D was recommended for $T_1 < tD < T_2$. For noncarcinogenic

COPCs, Equation 5-1E was recommended.

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U.S. EPA OSW recommends the use of Equations 5-1C, 5-1D, and 5-1E to calculate the cumulative soil concentration (*Cs*). The use of these equations is further described in Appendix B, Table B-1-1.

Recommended Equations for Calculating:
Cumulative Soil Concentration (*Cs*)

Carcinogens:

For $T_2 \leq tD$

$$Cs = \frac{Ds}{ks \cdot (tD - T_1)} \cdot \left[\left(tD + \frac{\exp\ (-ks \cdot tD)}{ks} \right) - \left(T_1 + \frac{\exp(-ks \cdot T_1)}{ks} \right) \right]$$
    Equation 5-1C

For $T_1 < tD < T_2$

$$Cs = \frac{(\dfrac{Ds \cdot tD - Cs_{tD}}{ks}) + (\dfrac{Cs_{tD}}{ks}) \cdot (1 - \exp\ [-ks \cdot (T_2 - tD)])}{(T_2 - T_1)}$$
    Equation 5-1D

Noncarcinogens:

$$Cs_{tD} = \frac{Ds \cdot [1 - \exp(-ks \cdot tD)]}{ks}$$
    Equation 5-1E

---

where

Cs	=	Average soil concentration over exposure duration (mg COPC/kg soil)
Ds	=	Deposition term (mg COPC/kg soil/yr)
T_1	=	Time period at the beginning of combustion (yr)
ks	=	COPC soil loss constant due to all processes (yr^{-1})
tD	=	Time period over which deposition occurs (time period of combustion) (yr)
Cs_{tD}	=	Soil concentration at time *tD* (mg/kg)
T_2	=	Length of exposure duration (yr)

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Consistent with U.S. EPA (1994r) and NC DEHNR (1997), when an exposure duration that is less than or equal to the operating lifetime of the emission source or hazardous waste combustion unit ($T_2 \leq tD$), Equation 5-1C is recommended; when an exposure duration greater than the operating lifetime of the hazardous waste combustion unit ($T_1 < tD < T_2$), Equation 5-1D is recommended. For noncarcinogenic COPCs, Equation 5-1E is recommended.

The COPC soil concentration averaged over the exposure duration, represented by Cs, should be used for carcinogenic compounds, where risk is averaged over the lifetime of an individual. Because the hazard quotient associated with noncarcinogenic COPCs is based on a reference dose rather than a lifetime exposure, the highest annual average COPC soil concentration occurring during the exposure duration period should be used for noncarcinogenic COPCs. The highest annual average COPC soil concentration, Cs_{tD}, will typically occur at the end of the operating life of the emission source or the time period of combustion.

Consistent with U.S. EPA (1994r) and NC DEHNR (1997), U.S. EPA OSW recommends using the highest 1-year annual average soil concentration, determined by using Equation 5-1E, to evaluate risk from noncarcinogenic COPCs (see Chapter 7).

5.2.2   Calculating the COPC Soil Loss Constant (*ks*)

Organic and inorganic COPCs may be lost from the soil by several processes that may or may not occur simultaneously. The rate at which a COPC is lost from the soil is known as the soil loss constant (*ks*). The constant *ks* is determined by using the soil's physical, chemical, and biological characteristics to consider the loss resulting from:

       (1)   leaching,

       (2)   runoff,

       (3)   erosion,

       (4)   biotic and abiotic degradation, and

       (5)   volatilization.

U.S. EPA (1990e) recommended the use of the following equation to calculate the soil loss constant (*ks*):

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$$ks = ksl + ksg + ksv \qquad\qquad \text{Equation 5-2}$$

where

ks	=	COPC soil loss constant due to all processes (yr^{-1})
ksl	=	COPC loss constant due to leaching (yr^{-1})
ksg	=	COPC loss constant due to biotic and abiotic degradation (yr^{-1})
ksv	=	COPC loss constant due to volatilization (yr^{-1})

U.S. EPA OSW recommends that Equation 5-2A be used to calculate the COPC soil loss constant (*ks*). This equation is further described in Appendix B, Table B-1-2. The use of Equation 5-2A is consistent with U.S. EPA (1993h), U.S. EPA (1994g), U.S. EPA (1994r), and NC DEHNR (1997).

Recommended Equation for Calculating:
COPC Soil Loss Constant (*ks*)

$$ks = ksg + kse + ksr + ksl + ksv \qquad\qquad \text{Equation 5-2A}$$

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where

ks	=	COPC soil loss constant due to all processes (yr^{-1})
ksg	=	COPC loss constant due to biotic and abiotic degradation (yr^{-1})
kse	=	COPC loss constant due to soil erosion (yr^{-1})
ksr	=	COPC loss constant due to surface runoff (yr^{-1})
ksl	=	COPC loss constant due to leaching (yr^{-1})
ksv	=	COPC loss constant due to volatilization (yr^{-1})

As highlighted in Section 5.2.1, the use of Equation 5-2A in Equations 5-1C and 5-1D assumes that COPC loss can be defined by using first-order reaction kinetics. First-order reaction rates depend on the concentration of one reactant (Bohn, McNeal, and O'Connor 1985). The loss of a COPC by a first-order process depends only on the concentration of the COPC in the soil, and a constant fraction of the COPC is removed from the soil over time. Those processes that apparently exhibit first-order reaction kinetics without implying a mechanistic dependence on a first-order loss rate are termed "apparent first-order"

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loss rates (Sparks 1989). The assumption that COPC loss follows first-order reaction kinetics may be an oversimplification because—at various concentrations or under various environmental conditions—the loss rates from soil systems will resemble different kinetic expressions. However, at low concentrations, a first-order loss constant may be adequate to describe the loss of the COPC from soil (U.S. EPA 1990e).

COPC loss in soil can also follow zero or second-order reaction kinetics. Zero-order reaction kinetics are independent of reactant concentrations (Bohn, McNeal, and O'Connor 1985). Zero-order loss rates describe processes in which the reactants are present at very high concentrations. Under zero-order kinetics, a constant amount of a COPC is lost from the soil over time, independent of its concentration. Processes that follow second-order reaction kinetics depend on the concentrations of two reactants or the concentration of one reactant squared (Bohn, McNeal, and O'Connor 1985). The loss constant of a COPC following a second-order process can be contingent on its own concentration, or on both its concentration and the concentration of another reactant, such as an enzyme or catalyst.

Because COPC loss from soil depends on many complex factors, it may be difficult to model the overall rate of loss. In addition, because the physical phenomena that cause COPC loss can occur simultaneously, the use of Equation 5-2A may also overestimate loss rates for each process (Valentine 1986). When possible, the common occurrence of all loss processes should be taken into account. Combined rates of soil loss by these processes can be derived experimentally; values for some COPCs are presented in U.S. EPA (1986c).

Sections 5.2.2.1 through 5.2.2.5 discuss issues associated with the calculation of the *ksl*, *kse*, *ksr*, *ksg*, and *ksv* variables.

5.2.2.1 COPC Loss Constant Due to Biotic and Abiotic Degradation *(ksg)*

Soil losses resulting from biotic and abiotic degradation (*ksg*) are determined empirically from field studies and should be addressed in the literature (U.S. EPA 1990e). Lyman et al. (1982) states that degradation rates can be assumed to follow first order kinetics in a homogenous media. Therefore, the half-life of a compound can be related to the degradation rate constant. Ideally, *ksg* is the sum of all biotic and abiotic rate constants in the soil media. Therefore, if the half-life of a compound (for all of the mechanisms of transformation) is known, the degradation rate can be calculated. However, literature sources do not provide sufficient data for all such mechanisms, especially for soil. U.S. EPA guidance

(1994g) had stated that *ksg* values for all COPCs other than 2,3,7,8-TCDD should be set equal to zero.

Appendix A-3 presents U.S. EPA OSW recommended values for this compound specific variable.

Recommended Values for:
COPC Loss Constant Due to Biotic and Abiotic Degradation (ksg)
See Appendix A-3

The rate of biological degradation in soils depends on the concentration and activity of the microbial populations in the soil, the soil conditions, and the COPC concentration (Jury and Valentine 1986). First-order loss rates often fail to account for the high variability of these variables in a single soil system. However, the use of simple rate expressions may be appropriate at low chemical concentrations (e.g., nanogram per kilogram soil) at which a first-order dependence on chemical concentration may be reasonable. The rate of biological degradation is COPC-specific, depending on the complexity of the COPC and the usefulness of the COPC to the microorganisms. Some substrates, rather than being used by the organisms as a nutrient or energy source, are simply degraded with other similar COPCs, which can be further utilized. Environmental and COPC-specific factors that may limit the biodegradation of COPCs in the soil environment (Valentine and Schnoor 1986) include:

  (1)   availability of the COPC,

  (2)   nutrient limitations,

  (3)   toxicity of the COPC, and

  (4)   inactivation or nonexistence of enzymes capable of degrading the COPC.

Chemical degradation of organic compounds can be a significant mechanism for removal of COPCs in soil (U.S. EPA 1990e). Hydrolysis and oxidation-reduction reactions are the primary chemical transformation processes occurring in the upper layers of soils (Valentine 1986). General rate expressions describing the transformation of some COPCs by all non-biological processes are available, and these expressions are helpful when division into component reactions is not possible.

Hydrolysis in aqueous systems is characterized by three processes: acid-catalyzed, base-catalyzed, and neutral reactions. The overall rate of hydrolysis is the sum of the first-order rates of these processes (Valentine 1986). In soil systems, sorption of the COPC can increase, decrease, or not affect the rate of

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hydrolysis, as numerous studies cited in Valentine (1986) have shown. The total rate of hydrolysis in soil can be predicted by adding the rates in the soil and water phases, which are assumed to be first-order reactions at a fixed pH (Valentine 1986). Methods for estimating these hydrolysis constants are described by Lyman et al. (1982).

Organic and inorganic compounds also undergo oxidation-reduction (redox) reactions in the soil (Valentine 1986). Organic redox reactions involve the exchange of oxygen and hydrogen atoms by the reacting molecules. Inorganic redox reactions may involve the exchange of atoms or electrons by the reactants. In soil systems where the identities of oxidant and reductant species are not specified, a first-order rate constant can be obtained for describing loss by redox reactions (Valentine 1986). Redox reactions involving metals may promote losses from surface soils by making metals more mobile (e.g., leaching to subsurface soils).

5.2.2.2 COPC Loss Constant Due to Soil Erosion (*kse*)

U.S. EPA (1993h) recommended the use of Equation 5-3 to calculate the constant for soil loss resulting from erosion (*kse*).

$$ kse \; = \; \frac{0.1 \cdot X_e \cdot SD \cdot ER}{BD \cdot Z_s} \cdot \frac{Kd_s \cdot BD}{\theta_{sw} + (Kd_s \cdot BD)} \qquad \text{Equation 5-3} $$

where

kse	=	COPC soil loss constant due to soil erosion
0.1	=	Units conversion factor (1,000 g-kg/10,000 cm^2-m^2)
X_e	=	Unit soil loss (kg/m^2-yr)
SD	=	Sediment delivery ratio (unitless)
ER	=	Soil enrichment ratio (unitless)
Kd_s	=	Soil-water partition coefficient (mL water/g soil)
BD	=	Soil bulk density (g soil/cm^3 soil)
Z_s	=	Soil mixing zone depth (cm)
θ_{sw}	=	Soil volumetric water content (mL water/cm^3 soil)

Unit soil loss (X_e) is calculated by using the Universal Soil Loss Equation (USLE) (See Section 5.7.2). Soil bulk density (*BD*) is described in Section 5.2.5.2. Soil volumetric water content (θ_{sw}) is described in

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Section 5.2.5.4. Site-specific variables associated with Equation 5-3 are further discussed in
Appendix B.

U.S. EPA guidance (1994g and 1994r) have stated that all *kse* values are equal to zero. U.S. EPA (1994r)
stated that *kse* is equal to zero because of contaminated soil eroding onto and off of the site.

Consistent with U.S. EPA guidance (1994g and 1994r), U.S. EPA OSW recommends that the constant
for the loss of soil resulting from erosion (*kse)* should be set equal to zero.

Recommended Value for: COPC Loss Constant Due to Erosion (*kse*)
0

For additional information on addressing *kse*, U.S. EPA OSW recommends consulting the methodologies
described in U.S. EPA NCEA document, *Methodology for Assessing Health Risks Associated with
Multiple Exposure Pathways to Combustor Emissions* (In Press). The use of *kse* values is also further
described in Appendix B, Table B-1-3.

5.2.2.3 COPC Loss Constant Due to Runoff (*ksr*)

Consistent with U.S. EPA (1993h; 1994r) and NC DEHNR (1997), U.S. EPA OSW recommends that
Equation 5-4 be used to calculate the constant for the loss of soil resulting from surface runoff (*ksr*). The
use of this equation is further described in Appendix B, Table B-1-4.

Recommended Equation for Calculating: COPC Loss Constant Due to Runoff (*ksr*)

$$ksr \; = \; \frac{RO}{\theta_{sw} \cdot Z_s} \cdot \left(\frac{1}{1 + \left(Kd_s \cdot BD / \theta_{sw} \right)} \right) \qquad\qquad \text{Equation 5-4}$$

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where

ksr	$=$	COPC loss constant due to runoff (yr^{-1})
RO	$=$	Average annual surface runoff from pervious areas (cm/yr)
θ_{sw}	$=$	Soil volumetric water content (mL water/cm^3 soil)
Z_s	$=$	Soil mixing zone depth (cm)
Kd_s	$=$	Soil-water partition coefficient (mL water/g soil)
BD	$=$	Soil bulk density (g soil/cm^3 soil)

Earlier U.S. EPA guidance (1994g) has stated that all *ksr* values should be set equal to zero. Soil bulk density (*BD*) is described in Section 5.2.5.2. Soil volumetric water content (θ_{sw}) is described in Section 5.2.5.4.

5.2.2.4 COPC Loss Constant Due to Leaching (*ksl*)

Losses of soil COPCs due to leaching (*ksl*) depend on the amount of water available to generate leachate and soil properties such as bulk density, soil moisture, soil porosity, and soil sorption properties.

U.S. EPA (1990e) recommended that Equation 5-5 be used to calculate the COPC loss constant due to leaching (*ksl*).

$$ksl \ = \ \frac{P + I - E_v}{\theta_{sw} \cdot Z_s \cdot [1.0 + (\ Kd_s \cdot BD \ /\theta_{sw}\ )]} \qquad\qquad \text{Equation 5-5}$$

where

ksl	$=$	COPC loss constant due to leaching (yr^{-1})
P	$=$	Average annual precipitation (cm/yr)
I	$=$	Average annual irrigation (cm/yr)
E_v	$=$	Average annual evapotranspiration (cm/yr)
θ_{sw}	$=$	Soil volumetric water content (mL water/cm^3 soil)
Z_s	$=$	Soil mixing zone depth (cm)
Kd_s	$=$	Soil-water partition coefficient (mL water/g soil)
BD	$=$	Soil bulk density (g soil/cm^3 soil)

U.S. EPA (1993h) determined that Equation 5-5 does not properly account for surface runoff. U.S. EPA (1994g) stated that all *ksl* values should be set equal to zero.

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More recent guidance (U.S. EPA 1993h; U.S. EPA 1994r; NC DEHNR 1997) have recommended

Equation 5-5A to calculate the COPC loss constant due to leaching. Consistent with U.S. EPA (1993h),

U.S. EPA (1994r), and NC DEHNR (1997), U.S. EPA OSW recommends that Equation 5-5A be used to

calculate the COPC loss constant due to leaching (*ksl*) to account for runoff. The use of this equation is

further described in Appendix B, Table B-1-5.

Recommended Equation for Calculating:
COPC Loss Constant Due to Leaching (*ksl*)

$$ksl = \frac{P + I - RO - E_v}{\theta_{sw} \cdot Z_s \cdot [1.0 + (BD \cdot Kd_s / \theta_{sw})]}$$

Equation 5-5A

---

where

ksl	=	COPC loss constant due to leaching (yr^{-1})
P	=	Average annual precipitation (cm/yr)
I	=	Average annual irrigation (cm/yr)
RO	=	Average annual surface runoff from pervious areas (cm/yr)
E_v	=	Average annual evapotranspiration (cm/yr)
θ_{sw}	=	Soil volumetric water content (mL water/cm^3 soil)
Z_s	=	Soil mixing zone depth (cm)
Kd_s	=	Soil-water partition coefficient (cm^3 water/g soil)
BD	=	Soil bulk density (g soil/cm^3 soil)

Appendix B describes the determination of site-specific variables associated with Equation 5-5A. The

average annual volume of water ($P + I - RO - E_v$) available to generate leachate is the mass balance of all

water inputs and outputs from the area under consideration. These variables are described in

Section 5.2.5.3. Soil bulk density (*BD*) is described in Section 5.2.5.2. Soil volumetric water content

(θ_{sw}) is described in Section 5.2.5.4.

5.2.2.5 COPC Loss Constant Due to Volatilization (*ksv*)

Semi-volatile and volatile COPCs emitted in high concentrations may become adsorbed to soil particles

and exhibit volatilization losses from soil. The loss of a COPC from the soil by volatilization depends on

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the rate of movement of the COPC to the soil surface, the chemical vapor concentration at the soil

surface, and the rate at which vapor is carried away by the atmosphere (Jury 1986).

U.S. EPA (1990e) recommended the use of Equation 5-6 to calculate the constant for the loss of soil

resulting from volatilization (*ksv*).

$$ksv = Ke \cdot Kt$$ Equation 5-6

where

ksv	=	COPC loss constant due to volatization (yr^{-1})
Ke	=	Equilibrium coefficient (s/cm-yr)
Kt	=	Gas phase mass transfer coefficient (cm/s)

U.S. EPA (1993h) did not identify a reference for Equation 5-6. However, U.S. EPA (1993h) stated that

Equation 5-6 had not been independently verified as accurately representing volatilization loss, but that

the equation for *Kt* (Equation 5-8) appeared to fit to data empirically. U.S. EPA (1993h) also stated that

ksv is modeled as a means of limiting soil concentration; because this mass flux never experiences rain

out, or washout and subsequent re-deposit, soil COPC concentrations are underestimated for soluble

volatile COPCs. U.S. EPA (1993h) recommended that the volatilized residues of semi-volatile COPCs

(such as dioxin) not be considered, but that additional research be conducted to determine the magnitude

of the uncertainty introduced for volatile COPCs. U.S. EPA (1994g) stated that all *ksv* values should be

set to zero.

U.S. EPA guidance (1994r) and NC DEHNR (1997) recommended calculating *ksv* values using

Equation 5-6A. Equation 5-6A appears to incorporate equations that U.S. EPA (1990e) recommended

for use in calculating *Ke* (equilibrium coefficient) and *Kt* (gas phase mass transfer coefficient).

$$ksv = \left(\frac{3.1536 \times 10^7 \cdot H}{Z_s \cdot Kd_s \cdot R \cdot T_a \cdot BD} \right) \cdot \left(0.482 \cdot W^{0.78} \cdot \left[\frac{\mu_a}{\rho_a \cdot D_a} \right]^{-0.67} \cdot \left[\sqrt{\frac{4 \cdot A}{\pi}} \right]^{-0.11} \right)$$ Equation 5-6A

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where

ksv	=	COPC loss constant due to volatization (yr^{-1})
3.1536×10^7	=	Units conversion factor (s/yr)
H	=	Henry's Law constant (atm-m^3/mol)
Z_s	=	Soil mixing zone depth (cm)
Kd_s	=	Soil-water partition coefficient (cm^3 water/g soil)
R	=	Universal gas constant (atm-m^3/mol-K)
T_a	=	Ambient air temperature (K) = 298.1 K
BD	=	Soil bulk density (g soil/cm^3 soil)
0.482	=	Empirical constant (unitless)
W	=	Average annual wind speed (m/s)
μ_a	=	Viscosity of air (g/cm-s)
ρ_a	=	Density of air (g/cm^3)
D_a	=	Diffusivity of COPC in air (cm^2/s)
A	=	Surface area of contaminated area (m^2)
0.78	=	Empirical constant (unitless)
-0.67	=	Empirical constant (unitless)
-0.11	=	Empirical constant (unitless)
0.482	=	Units conversion factor [(3600 s/hr)$^{0.78}$(100 cm/m)/(3600 s/hr)] · (empirical constant 0.0292)

U.S. EPA (1990e) recommended that Equation 5-7 be used to calculate *Ke* and Equation 5-8 be used to calculate *Kt*.

$$Ke = \frac{3.1536 \times 10^7 \cdot (H \times 10^3)}{Z_s \cdot Kd_s \cdot R \cdot T_a \cdot BD}$$

Equation 5-7

$$Kt = 0.482 \cdot W^{0.78} \cdot Sc_a^{-0.67} \cdot d_e^{-0.11}$$

Equation 5-8

where

Ke	=	Equilibrium coefficient (s/cm-yr)
3.1536×10^7	=	Units conversion factor (s/yr)
H	=	Henry's Law constant (atm-L/mol)
10^3	=	Units conversion factor (L/m^3)
Z_s	=	Soil mixing zone depth (cm)
Kd_s	=	Soil-water partition coefficient (cm^3 water/g soil)
R	=	Universal gas constant (atm-m^3/mol-K)
T_a	=	Ambient air temperature (K) = 298.1 K
BD	=	Soil bulk density (g soil/cm^3 soil)

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Kt	=	Gas phase mass transfer coefficient (cm/s)
W	=	Average annual wind speed (m/s)
Sc_a	=	Schmidt number for gas phase (unitless)
d_e	=	Effective diameter of contaminated media (m)
0.482	=	Units conversion factor $[(3600 \text{ s/hr})^{0.78}(100 \text{ cm/m})/(3600 \text{ s/hr})] \cdot$ (empirical constant 0.0292)

Equations 5-9 and 5-10 are used to calculate the Schmidt number for gas phase (Sc_a) and the effective diameter of contaminated media (d_e) respectively (U.S. EPA 1990e).

$$Sc_a = \frac{\mu_a}{\rho_a \cdot D_a}$$

Equation 5-9

$$d_e = \sqrt{\frac{4 \cdot A}{\pi}}$$

Equation 5-10

where

Sc_a	=	Schmidt number for gas phase (unitless)
μ_a	=	Viscosity of air (g/cm-s)
ρ_a	=	Density of air (g/cm^3)
D_a	=	Diffusivity of COPC in air (cm^2/s)
d_e	=	Effective diameter of contaminated media (m)
A	=	Surface area of contaminated area (m^2)

Consistent with U.S. EPA guidance (1994g) and based on the need for additional research to be conducted to determine the magnitude of the uncertainty introduced for modeling volatile COPCs from soil, U.S. EPA OSW recommends that, until identification and validation of more applicable models, the constant for the loss of soil resulting from volatilization (*ksv*) should be set equal to zero.

Recommended Value for: COPC Loss Constant Due to Volatilization (*ksv*)
0

In cases where high concentrations of volatile organic compounds are expected to be present in the soil, U.S. EPA OSW recommends consulting the methodologies described in U.S. EPA NCEA document,

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Methodology for Assessing Health Risks Associated with Multiple Exposure Pathways to Combustor

Emissions (In Press). The use of *ksv* values is also further described in Appendix B, Table B-1-6.

5.2.3   Calculating the Deposition Term (*Ds*)

U.S. EPA OSW recommends that Equation 5-11 be used to calculate the deposition term *(Ds)*. This

equation is further described in Appendix B, Table B-1-1. The use of Equation 5-11 to calculate the

deposition term is consistent with U.S. EPA (1994r) and NC DEHNR (1997), which both incorporate a

deposition term (*Ds*) into Equation 5-1C.

Recommended Equation for Calculating:
Deposition Term (*Ds*)

$$Ds = \left[\frac{100 \cdot Q}{Z_s \cdot BD}\right] \cdot [F_v \cdot (0.31536 \cdot Vdv \cdot Cyv + Dywv) + (Dydp + Dywp) \cdot (1 - F_v)] \quad \text{Equation 5-11}$$

---

where

Ds	=	Deposition term (mg COPC/kg soil/yr)
100	=	Units conversion factor (mg-m^2/kg-cm^2)
Q	=	COPC emission rate (g/s)
Z_s	=	Soil mixing zone depth (cm)
BD	=	Soil bulk density (g soil/cm^3 soil)
F_v	=	Fraction of COPC air concentration in vapor phase (unitless)
0.31536	=	Units conversion factor (m-g-s/cm-µg-yr)
Vdv	=	Dry deposition velocity (cm/s)
Cyv	=	Unitized yearly average air concentration from vapor phase (mg-s/g-m^3)
Dywv	=	Unitized yearly average wet deposition from vapor phase (s/m^2-yr)
Dydp	=	Unitized yearly average dry deposition from particle phase (s/m^2-yr)
Dywp	=	Unitized yearly average wet deposition from particle phase (s/m^2-yr)

Chapter 3 describes determination of modeled air parameters *Cyv*, *Dywv*, *Dydp*, and *Dywp*. Appendix B

describes determination of the site-specific parameters associated with Equation 5-11. Appendix A-3

describes determination of the compound-specific parameter *Fv*.

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5.2.4   Universal Soil Loss Equation (USLE)

U.S. EPA OSW recommends that the universal soil loss equation (USLE) be used to calculate the unit soil loss *(X_e)*. This equation is further described in Section 5.7.2 and in Appendix B, Table B-4-13.

5.2.5   Site-Specific Parameters for Calculating Cumulative Soil Concentration

Calculating average soil concentration over the exposure duration (*Cs*) requires the use of site-specific parameters including the following:

- Soil mixing zone depth (Z_s)

- Soil bulk density (*BD*)

- Available water ($P + I - RO - E_v$)

- Soil volumetric water content (q_{sw})

Determination of values for these parameters is further described in the following subsections, and in Appendix B.

5.2.5.1 Soil Mixing Zone Depth (Z_s)

When exposures to COPCs in soils are modeled, the depth of contaminated soils is important in calculating the appropriate soil concentration. COPCs deposited onto soil surfaces may be moved into lower soil profiles by tilling, whether manually in a garden or mechanically in a large field.

In general, U.S. EPA (1990e) and U.S. EPA (1992d) have estimated that if the area under consideration is likely to be tilled, soil depth is about 10 to 20 centimeters depending on local conditions and the equipment used. If soil is not moved, COPCs are assumed to be retained in the shallower, upper soil layer. In this case, earlier U.S. EPA guidances (U.S. EPA 1990e; U.S. EPA 1993h) have typically recommended a value of 1 centimeter.

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The assumption made to determine the value of Z_s may affect the outcome of the risk assessment, because soil concentrations that are based on soil depth are used to calculate exposure via several pathways:

(1)   ingestion of plants contaminated by root uptake and by volatilization from soil;

(2)   direct ingestion of soil by humans, cattle, swine, or chicken; and

(3)   surface runoff into water bodies.

For example, in calculations of exposures resulting from uptake through plant roots, the average concentration of COPCs over the depth of the plant root determines plant uptake. However, in calculations of plant uptake resulting from volatilization, only the uppermost soil layer is considered.

U.S. EPA (1990e) recommended that soil mixing depths be selected as follows:

Soil Depth (Z_s)	Exposure	Description
1 cm	Direct ingestion of soil	Human exposure: in gardens, lawns, landscaped areas, parks, and recreational areas. Animal exposure: in pastures, lawns, and parks (untilled soils).
1 cm	Surface water runoff in nonagricultural areas	These areas are typically assumed to be untilled.
20 cm	Plant uptake for agricultural soils	The root depth is assumed to equal the tilling depth of 20 centimeters. In untilled soils, the root zone does not directly reflect tilling depth, although it is assumed that tilling depth is an adequate substitute for root zone depth.
20 cm	Surface water runoff in agricultural areas	These areas are typically assumed to be tilled.

Consistent with U.S. EPA (1990e), U.S. EPA OSW recommends the following values for the soil mixing zone depth (Z_s).

Recommended Values for: **Soil Mixing Zone Depth (Z_s)**
1 cm - untilled   20 cm - tilled

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U.S. EPA guidance (1990e) stated that any volatile COPCs are not likely to be associated with particulates soon after emission from the combustion unit; before deposition onto the soil. However, semi-volatile COPCs and volatile COPCs emitted in sufficiently high concentrations may be deposited in particulate form and exhibit volatilization losses from soils. COPCs subject to volatilization losses may be moved to 20 centimeters by tilling and will not readily volatilize from this depth. The volatilization rate will reflect only the COPC concentration at the soil surface.

5.2.5.2 Soil Dry Bulk Density (*BD*)

BD is the ratio of the mass of soil to its total volume. This variable is affected by the soil structure, type, and moisture content (Hillel 1980). Consistent with U.S. EPA (1990e; 1994g) and presented in Hoffman and Baes (1979), U.S. EPA OSW recommends the following value for the soil dry bulk density (*BD*).

Recommended Value for: Soil Dry Bulk Density (*BD*)
1.50 g/cm^3

U.S. EPA (1994r) recommended that wet soil bulk density be determined by weighing a thin-walled, tube soil sample (e.g., a Shelby tube) of known volume and subtracting the tube weight (ASTM Method D2937). Moisture content can then be calculated (ASTM Method 2216) to convert wet soil bulk density to dry soil bulk density.

5.2.5.3 Available Water (*P + I - RO - E$_v$*)

The average annual volume of water available (*P + I - RO - E$_v$*) for generating leachate is the mass balance of all water inputs and outputs from the area under consideration. A wide range of values for these site-specific parameters may apply in the various U.S. EPA regions.

The average annual precipitation (*P*), irrigation (*I*), runoff (*RO*), and evapotranspiration (*E$_v$*) rates and other climatological data may be obtained from either data recorded on site or from the Station Climatic Summary for a nearby airport.

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Meteorological variables—such as the evapotranspiration rate (E_v) and the runoff rate (RO)—may also be found in resources such as Geraghty, Miller, van der Leeden, and Troise (1973). Surface runoff may also be estimated by using the Curve Number Equation developed by the U.S. Soil Conservation Service (U.S. EPA 1990e). U.S. EPA (1985b) cited isopleths of mean annual cropland runoff corresponding to various curve numbers developed by Stewart, Woolhiser, Wischmeier, Caro, and Frere (1975). Curve numbers are assigned to an area on the basis of soil type, land use or cover, and the hydrologic conditions of the soil (U.S. EPA 1990e).

Using these different references, however, introduces uncertainties and limitations. For example, Geraghty, Miller, van der Leeden, and Troise (1973) presented isopleths for annual surface water contributions that include interflow and ground water recharge. As noted in U.S. EPA (1994g), these values should be adjusted downward to reflect surface runoff only. U.S. EPA (1994g) recommended that these values be reduced by 50 percent.

5.2.5.4 Soil Volumetric Water Content (θ_{sw})

The soil volumetric water content (θ_{sw}) depends on the available water and the soil structure. A wide range of values for these variables may apply in the various U.S. EPA regions. Consistent with earlier guidance documents, (U.S. EPA 1993k; U.S. EPA 1994g; NC DEHNR 1977), U.S. EPA OSW recommends a value for θ_{sw} of 0.2 ml/cm^3.

Recommended Value for: Soil Volumetric Water Content (θ_{sw})
0.2 ml/cm^3

5.3   CALCULATION OF COPC CONCENTRATIONS IN PRODUCE

Indirect exposure resulting from ingestion of produce depends on the total concentration of COPCs in the leafy, fruit, and tuber portions of the plant. Because of general differences in contamination mechanisms, consideration of indirect exposure separates produce into two broad categories—aboveground produce and belowground produce. In addition, aboveground produce should

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be further subdivided into exposed and protected aboveground produce for consideration of
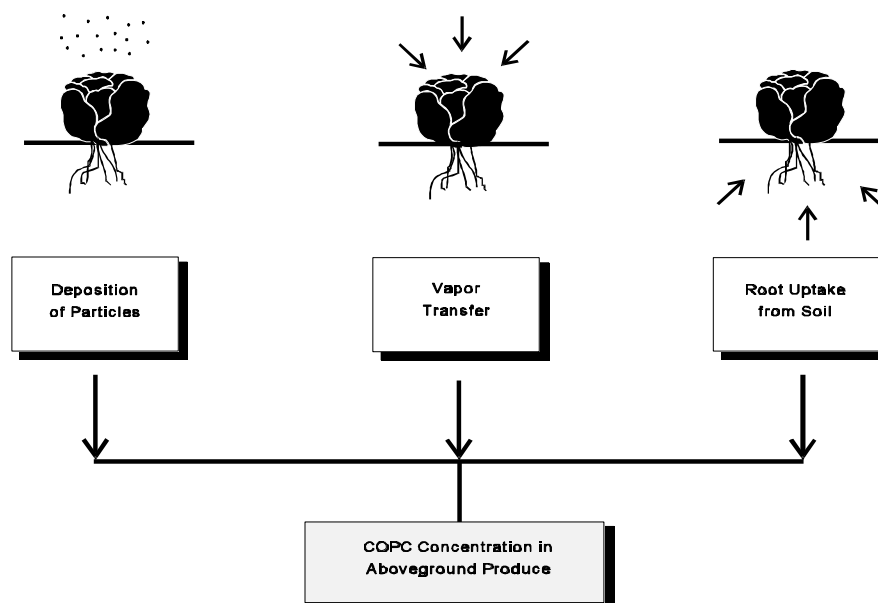
contamination as a result of indirect exposure.

Figure 5-3 COPC Concentration in Produce

Aboveground Produce

Aboveground exposed produce is assumed to be contaminated by three possible mechanisms:

- **Direct deposition of particles**—wet and dry deposition of particle phase COPCs on the leaves and fruits of plants (Section 5.3.1).

- **Vapor transfer**—uptake of vapor phase COPCs by plants through their foliage (Section 5.3.2).

- **Root uptake**—root uptake of COPCs available from the soil and their transfer to the aboveground portions of the plant (Section 5.3.3).

The total COPC concentration in aboveground exposed produce is calculated as a sum of contamination

occurring through all three of these mechanisms. However, edible portions of aboveground protected

produce, such as peas, corn, and melons, are covered by a protective covering; hence, they are protected

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from contamination through deposition and vapor transfer. Therefore, root uptake of COPCs is the primary mechanism through which aboveground protected produce becomes contaminated (Section 5.3.3). Appendix B further describes the equations and parameters used to calculate COPC concentrations in exposed and protected aboveground produce.

Belowground Produce

For belowground produce, contamination is assumed to occur only through one mechanism—root uptake of COPCs available from soil (Section 5.3.3). Contamination of belowground produce via direct deposition of particles and vapor transfer are not considered because the root or tuber is protected from contact with contaminants in the vapor phase. Appendix B further describes the equations and parameters used to calculate COPC concentrations in belowground produce.

Generally, risks associated with exposure of VOCs via food-chain pathways have not been considered significant, primarily because VOCs are typically low-molecular-weight COPCs that do not persist in the environment and do not bioaccumulate (U.S. EPA 1994r; U.S. EPA 1996g). However, as discussed in Chapter 2, U.S. EPA OSW recommends that all COPCs, including VOCs, be evaluated for each exposure pathway.

5.3.1   Aboveground Produce Concentration Due to Direct Deposition (*Pd*)
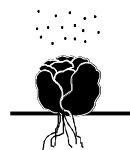
Earlier guidance documents (U.S. EPA [1990e]) and U.S. EPA [1993h]) proposed that COPC concentrations in aboveground vegetation resulting from wet and dry deposition onto plant surfaces of leafy plants and exposed produce (*Pd*) be calculated as follows:

$$Pd_i = \frac{1{,}000 \cdot [Dyd + (Fw \cdot Dyw)] \cdot Rp_i \cdot [1.0 - \exp(-kp \cdot Tp_i)]}{Yp_i \cdot kp} \qquad \text{Equation 5-13}$$

where

Pd_i	=	Concentration of pollutant due to direct deposition in the *i*th plant group (μg COPC/g plant tissue DW))
1,000	=	Units conversion factor (kg/10^3 g and 10^6 μg/g pollutant)
Dyd	=	Yearly dry deposition from particle phase (g/m^2-yr)
Fw	=	Fraction of COPC wet deposition that adheres to plant surfaces (unitless)

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Dyw	=	Yearly wet deposition from vapor phase (g/m^2-yr)
Rp_i	=	Interception fraction of the edible portion of plant tissue for the ith plant group (unitless)
kp	=	Plant surface loss coefficient (yr^{-1})
Tp_i	=	Length of plant's exposure to deposition per harvest of the edible portion of the ith plant group (yr)
Yp_i	=	Yield or standing crop biomass of edible portion of the ith plant group (kg DW/m^2)

U.S. EPA (1994r) modified Equation 5-13 to include stack emissions adjusted to remove the fraction of air concentration in vapor phase [$Q (1 - F_v)$] (Equation 5-14).

U.S. EPA OSW recommends the use of Equation 5-14 to calculate COPC concentration in exposed and aboveground produce due to direct deposition. The use of this equation is further described in Appendix B, Table B-2-7.

Recommended Equation for Calculating:
Aboveground Produce Concentration Due to Direct Deposition (Pd)

$$Pd = \frac{1,000 \cdot Q \cdot (1 - F_v) \cdot [Dydp + (Fw \cdot Dywp)] \cdot Rp \cdot [1.0 - \exp(-kp \cdot Tp)]}{Yp \cdot kp}$$ Equation 5-14

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where

Pd	=	Plant (aboveground produce) concentration due to direct (wet and dry) deposition (mg COPC/kg DW)
1,000	=	Units conversion factor (mg/g)
Q	=	COPC emission rate (g/s)
F_v	=	Fraction of COPC air concentration in vapor phase (unitless)
$Dydp$	=	Unitized yearly average dry deposition from particle phase (s/m^2-yr)
Fw	=	Fraction of COPC wet deposition that adheres to plant surfaces (unitless)
$Dywp$	=	Unitized yearly wet deposition from particle phase (s/m^2-yr)
Rp	=	Interception fraction of the edible portion of plant (unitless)
kp	=	Plant surface loss coefficient (yr^{-1})
Tp	=	Length of plant exposure to deposition per harvest of the edible portion of the ith plant group (yr)

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| *Yp* | = | Yield or standing crop biomass of the edible portion of the plant (productivity) (kg DW/m^2) |

Chapter 3 describes the determination of the modeled air parameters *Dydp* and *Dywp*. Appendix A-3 describes determination of *Fv*. Appendix B describes determination of *Fw*. *Rp*, *kp*, *Tp*, and *Yp* are neither site- nor COPC-specific, and are described in Sections 5.3.1.1 through 5.3.1.4.

5.3.1.1 Interception Fraction of the Edible Portion of Plant (*Rp*)

U.S. EPA (1990e) stated that NRC models assumed a constant of 0.2 for *Rp* for dry and wet deposition of particles (Boone, Ng, and Palm 1981). However, Shor, Baes, and Sharp (1982) suggested that diversity of plant growth necessitated vegetation-specific *Rp* values.

As summarized in Baes, Sharp, Sjoreen, and Shor (1984), experimental studies of pasture grasses identified a correlation between initial *Rp* values and productivity (standing crop biomass [*Yp*]) (Chamberlain 1970):

$$Rp \quad = \quad 1 - e^{-\gamma Yp} \qquad\qquad\qquad \text{Equation 5-14A}$$

where

Rp	=	Interception fraction of the edible portion of plant (unitless)
γ	=	Empirical constant (Chamberlain [1970] gives the range as 2.3 to 3.3 for pasture grasses; Baes, Sharp, Sjoreen, and Shor [1984] used the midpoint, 2.88, for pasture grasses.)
Yp	=	Standing crop biomass (productivity) (kg DW/m^2 for silage; kg WW/m^2 for exposed produce)

Baes, Sharp, Sjoreen, and Shor (1984) also developed methods for estimating *Rp* values for leafy vegetables, silage, and exposed produce. However, these vegetation class-specific calculations produced *Rp* values that were independent of productivity measurements. This independence led to potentially unreasonable estimates of surface plant concentrations. Therefore, Baes, Sharp, Sjoreen, and Shor (1984) proposed using the same empirical relationship developed by Chamberlain (1970) for other vegetation classes. Class-specific estimates of the empirical constant (γ) were developed by forcing an exponential regression equation through several points, including average and theoretical maximum

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estimates of *Rp* and *Yp* (Baes, Sharp, Sjoreen, and Shor 1984). Class-specific empirical constants (γ)

that were developed include the following:

- Exposed produce   =   0.0324

- Leafy vegetables   =   0.0846

- Silage   =   0.769

U.S. EPA (1994r) and U.S. EPA (1995e) proposed a default aboveground produce *Rp* value of 0.05,

which is based on a weighted average class-specific *Rp* values. Specifically, class-specific *Rp* values

were calculated by using the equation developed by Chamberlain (1970) and the following empirical

constants:

- Leafy vegetables were assigned the same empirical constant (0.0846) developed by Baes, Sharp, Sjoreen, and Shor (1984).

- Fruits, fruiting vegetables, and legumes were assigned the empirical constant (0.0324) originally developed by Baes, Sharp, Sjoreen, and Shor (1984) for "exposed produce."

Vegetables and fruits included in each class are as follows:

- Fruits—apple, apricot, berry, cherry, cranberry, grape, peach, pear, plum/prune, and strawberry

- Fruiting Vegetables—asparagus, cucumber, eggplant, sweet pepper, and tomato

- Legumes—snap beans

- Leafy Vegetables—broccoli, brussel sprouts, cauliflower, celery, lettuce, and spinach

The class-specific *Rp* values were then weighted by relative ingestion of each class to determine a

weighted average *Rp* value of 0.05. However, the produce classes and relative ingestion values used by

U.S. EPA (1994r) and U.S. EPA (1995e) to calculate and weight the *Rp* values are not current with the

U.S. EPA *1997 Exposure Factors Handbook* (U.S. EPA 1997c). In addition, the overall *Rp* value

presented in U.S. EPA (1994r; 1995e) was based on limited information; subsequent revision to U.S.

EPA (1994r; 1995e) has resulted in an overall *Rp* value of 0.2 (RTI 1997).

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For purposes of consistency, the produce classes have been combined into two groups—exposed fruit and exposed vegetables. The exposed produce empirical constant (γ) was used to calculate Rp. Since the exposed vegetable category includes leafy and fruiting vegetables, Rp was calculated for leafy and fruiting vegetables. The exposed vegetable Rp was then determined by a weighted average based on productivity (Yp) of leafy and fruiting vegetables, respectively. The relative ingestion rates used to determine an average weighted Rp value were derived from the intake of homegrown produce discussion presented in the 1997 *Exposure Factors Handbook* (U.S. EPA 1997c). U.S. EPA recommends the use of the weighted average Rp value of 0.39 as a default Rp value because it represents the most current parameters including standing crop biomass and relative ingestion rates.

Recommended Value for: Interception Fraction of the Edible Portion of Plant (Rp)
0.39

Unweighted Rp and ingestion rates used for the weighting were as follows:

Aboveground Produce Class	Rp	Ingestion Rate (g DW/kg-day)
Exposed fruits	0.053	0.19
Exposed vegetables	0.982	0.11

One of the primary uncertainties associated with this variable is whether the algorithm developed by Chamberlain (1970) and the empirical constants developed by Baes, Sharp, Sjoreen, and Shor (1984) for use in this algorithm accurately represent aboveground produce. Specifically, Chamberlain (1970) based his algorithm on studies of pasture grass rather than aboveground produce. Baes, Sharp, Sjoreen, and Shor (1984) noted that their approach to developing class-specific Rp values is "at best *ad hoc*," but stated that this approach was justified, because the consequences of using Rp estimates that are independent of productivity are "serious."

5.3.1.2 Plant Surface Loss Coefficient (kp)

U.S. EPA (1990e) identified several processes—including wind removal, water removal, and growth dilution—that reduce the amount of contaminant that has deposited on plant surfaces. The term kp is a measure of the amount of contaminant that is lost to these physical processes over time. U.S. EPA

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(1990e) cited Miller and Hoffman (1983) for the following equation:

$$kp = \left(\frac{\ln 2}{t_{1/2}} \right) \cdot 365$$
<div align="right">Equation 5-15</div>

where

kp	=	Plant surface loss coefficient (yr^{-1})
$t_{1/2}$	=	Half-life (days)
365	=	Units conversion factor (days/yr)

Miller and Hoffman (1983) reported half-life values ranging from 2.8 to 34 days for a variety of contaminants on herbaceous vegetation. These half-life values converted to kp values of 7.44 to 90.36 (yr^{-1}). U.S. EPA (1993h; 1994r) recommended a kp value of 18, based on a generic 14-day half-life corresponding to physical processes only. The 14-day half-life is approximately the midpoint of the range (2.8 to 34 days) estimated by Miller and Hoffman (1983).

U.S. EPA OSW recommends use of a plant surface loss coefficient (kp) value of 18. This kp value is the midpoint of Miller and Hoffman's (1983) range of values. Based on this range (7.44 to 90.36), plant concentrations could range from about 1.8 times higher to about 48 times lower than the plant concentrations, based on a kp value of 18.

Recommended Value for: Plant Surface Loss Coefficient (*kp*)
18

The primary uncertainty associated with this variable is that the calculation of kp does not consider chemical degradation processes. However, information regarding chemical degradation of contaminants on plant surfaces is limited. The inclusion of chemical degradation processes would result in decreased half-life values and thereby increase kp values. Note that effective plant concentration decreases as kp increases. Therefore, use of a kp value that does not consider chemical degradation processes is conservative. In addition, there are uncertainties associated with the half-life values reported by Miller and Hoffman (1983) with regard to how accurately these values represent the behavior of risk assessment

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COPCs on aboveground produce. However, the relative impact of this second uncertainty is less than the omission of chemical degradation processes.

5.3.1.3 Length of Plant Exposure to Deposition per Harvest of Edible Portion of Plant (*Tp*)

U.S. EPA (1990e), U.S. EPA (1993h), U.S. EPA (1994r), and NC DEHNR (1997) recommended treating *Tp* as a constant, based on the average period between successive hay harvests. This period was estimated at 60 days (0.164 years) by Belcher and Travis (1989) and represents the length of time that aboveground vegetation (in this case, hay) would be exposed to contaminant deposition before being harvested. *Tp* is calculated as follows:

$$Tp = \frac{60\ days}{365\ days/yr} = 0.164\ yr$$

Equation 5-16

where

Tp	=	Length of plant exposure to deposition per harvest of the edible portion of plant (yr)
60	=	Average period between successive hay harvests (days)
365	=	Units conversion factor (days/yr)

Consistent with previous guidance, U.S. EPA OSW recommends using a *Tp* value of 0.164 year as the best available default value.

Recommended Value for:
Length of Plant Exposure to Deposition per Harvest of Edible Portion of Plant (*Tp*)

0.164 years

The primary uncertainty associated with the use of this value is that it is based on the growing season for hay rather than aboveground produce. The average period between successive hay harvests (60 days) may not reflect the length of the growing season or the period between successive harvests for aboveground produce at specific sites. To the extent that information documenting the growing season or period between successive harvests for aboveground produce is available, this information may be used to estimate a site-specific *Tp* value. Calculated plant concentrations will be affected most if the site-specific value of *Tp* is significantly less than 60 days.

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5.3.1.4 Standing Crop Biomass (Productivity) (*Yp*)

U.S. EPA (1990e) stated that the best estimate of *Yp* is productivity, which Baes, Sharp, Sjoreen, and
Shor (1984) and Shor, Baes, and Sharp (1982) define as follows:

$$Yp \ = \ \frac{Yh_i}{Ah_i}$$

Equation 5-17

where

Yh_i	=	Harvest yield of the *i*th crop (kg DW)
Ah_i	=	area planted to the *i*th crop (m^2)

U.S. EPA (1994r) and NC DEHNR (1997) recommend using this equation and calculate *Yp* value of 1.6
for aboveground produce, based on weighted average *Yh* and *Ah* values for four aboveground produce
classes (fruits, fruiting vegetables, legumes, and leafy vegetables). Vegetables and fruits included in
each class are as follows:

- Fruits—apple, apricot, berry, cherry, cranberry, grape, peach, pear, plum/prune, and
  strawberry

- Fruiting Vegetables—asparagus, cucumber, eggplant, sweet pepper, and tomato

- Legumes—snap beans

- Leafy Vegetables—broccoli, brussel sprouts, cauliflower, celery, lettuce, and spinach.

Class-specific *Yp* values were estimated by using U.S. average *Yh* and *Ah* values for a variety of fruits
and vegetables for 1993 (USDA 1994a; USDA 1994b). *Yh* values were converted to dry weight by using
average class-specific conversion factors (Baes, Sharp, Sjoreen, and Shor 1984). U.S. EPA (1994r) and
U.S. EPA (1995e) calculated class-specific *Yp* values and then used relative ingestion rates of each group
to determine the weighted average *Yp* value of 1.6. However, the produce classes and relative ingestion
values used by U.S. EPA (1994r) and U.S. EPA (1995e) to calculate and weight the *Yp* values are not
current with the U.S. EPA 1997 *Exposure Factors Handbook*. In addition, overall *Yp* value presented in

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U.S. EPA (1994r) and U.S. EPA (1995e) was based on limited information; subsequent revision to

U.S. EPA (1994r) and U.S. EPA (1995e) has resulted in an overall *Yp* value of 1.7 (RTI 1997).

For consistency, the produce classes have been combined into two groups—exposed fruit and exposed

vegetables. The exposed vegetable *Yp* was determined by summing *Yh* values for leafy and fruiting

vegetables and dividing by the sum of *Ah* values for leafy and fruiting vegetables. The relative ingestion

rates used to determine an overall average weighted *Yp* value were derived from the homegrown produce

discussions presented in the 1997 *Exposure Factors Handbook* (U.S. EPA 1997c). U.S. EPA

recommends the use of the weighted average *Yp* value of 2.24 as a default *Yp* value based on this value

representing the most complete and thorough information available.

Recommended Value for: **Standing Crop Biomass (Productivity) (*Yp*)**
2.24

Unweighted *Yp* and ingestion rates used for the weighting were as follows:

Aboveground Produce Class	*Yp*	Ingestion Rate (g DW/kg-day)
Exposed fruits	0.25	0.19
Exposed vegetables	5.66	0.11

The primary uncertainty associated with this variable is that the harvest yield (*Yh*) and area planted (*Ah*)

may not reflect site-specific conditions. To the extent to which site-specific information is available, the

magnitude of the uncertainty introduced by the default *Yp* value can be estimated.

5.3.2   Aboveground Produce Concentration Due to Air-to-Plant Transfer (*Pv*)

The methodology used to estimate COPC concentration in exposed and aboveground produce

due to air-to-plant transfer (*Pv*) considers limitations of COPCs concentrations to transfer from

plant surfaces to the inner portions of the plant. These limitations result from mechanisms

responsible for inhibiting the transfer of the lipophilic COPC (e.g., the shape of the produce) and the

removal of the COPCs from the edible portion of the produce (e.g., washing, peeling, and cooking).

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U.S. EPA OSW recommends the use of Equation 5-18 to calculate aboveground produce concentration

due to air-to-plant transfer (*Pv*). The use of this equation is further described in Appendix B,

Table B-2-8.

Recommended Equation for Calculating:
Aboveground Produce Concentration Due to Air-to-Plant Transfer (*Pv*)

$$Pv \ = \ Q \cdot F_v \cdot \frac{Cyv \cdot Bv_{ag} \cdot VG_{ag}}{\rho_a}$$ Equation 5-18

---

where

Pv	=	Concentration of COPC in the plant resulting from air-to-plant transfer (μg COPC/g DW)
Q	=	COPC emission rate (g/s)
F_v	=	Fraction of COPC air concentration in vapor phase (unitless)
Cyv	=	Unitized yearly average air concentration from vapor phase (μg-s/g-m^3)
Bv_{ag}	=	COPC air-to-plant biotransfer factor ([mg COPC/g DW plant]/[mg COPC/g air]) (unitless)
VG_{ag}	=	Empirical correction factor for aboveground produce (unitless)
ρ_a	=	Density of air (g/m^3)

Chapter 3 describes the determination of the modeled air parameter *Cyv*. Appendix A-3 describes

determination of *Fv* and Bv_{ag}. Appendix B further describes use of Equation 5-18, including

determination of *Fw* and ρ_a. As discussed below in Section 5.3.2.1, the parameter VG_{ag} is dependent on

lipophilicity of the COPC, and assigned a value of 0.001 for lipophilic COPCs (log K_{ow} greater than 4) or

a value of 1.0 for COPCs with a log K_{ow} less than 4.

5.3.2.1 Empirical Correction Factor for Aboveground Produce (*VG$_{ag}$*)

The parameter VG_{ag} has been incorporated into Equation 5-18 to address the potential overestimation for

lipophilic COPCs to be transferred to the inner portions of bulky produce, such as apples. Because of the

protective outer skin, size, and shape of bulky produce, transfer of lipophilic COPCs (log K_{ow} greater

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than 4) to the center of the produce is not as likely as for non-lipophilic COPCs and, as a result, the inner

portions will be less affected.

To address this issue, U.S. EPA (1994m) recommended an empirical correction factor (VG_{ag}) of 0.01 for

lipophilic COPCs to reduce estimated vegetable concentrations. The factor of 0.01 is based on a similar

correction factor ($VG_{rootveg}$) for belowground produce, which is estimated for unspecified vegetables as

follows:

$$VG_{rootveg} = \frac{M_{skin}}{M_{vegetable}}$$ Equation 5-19

where

$VG_{rootveg}$ =   Correction factor for belowground produce (g/g)
M_{skin} =   Mass of a thin (skin) layer of belowground vegetable (g)
$M_{vegetable}$ =   Mass of the entire vegetable (g)

If it is assumed that the density of the skin and the whole vegetable are the same, this equation can

become a ratio of the volume of the skin to that of the whole vegetable. U.S. EPA (1994m) assumed that

the vegetable skin is 0.03 centimeters, which is the leaf thickness of a broad-leaf tree, as was used in

experiments conducted by Riederer (1990). With this assumption, U.S. EPA (1994m) calculated $VG_{rootveg}$

values of 0.09 and 0.03 for carrots and potatoes, respectively.

Based on the work by Wipf, Homberger, Neuner, Ranalder, Vetter, and Vuilleumier (1982), U.S. EPA

(1994m) identified other processes—such as peeling, cooking, and cleaning—that will further reduce the

vegetable concentration. U.S. EPA (1994m) recommended a $VG_{rootveg}$ value of 0.01 for lipophilic COPCs,

which is less than the aforementioned estimates of 0.09 and 0.03 for the carrot and potato, but greater

than the estimate would be if the correction factor was adjusted for cleaning, washing, and peeling, as

described by Wipf, Homberg, Neuner, Ranalder, Vetter, and Vuilleumier (1982). Following this line of

reasoning, U.S. EPA (1994m) recommended a lipophilic COPC VG_{ag} value of 0.01 for all aboveground

produce except leafy vegetables. As with $VG_{rootveg}$, U.S. EPA (1994m) noted that assignment of this value

is based on the consideration that it "should be less than estimated just based on surface volume to whole

fruit volume ratios."

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U.S. EPA (1994m) recommends a lipophilic COPC VG_{ag} of 1.0 for pasture grass because of a direct analogy to exposed azalea and grass leaves. Pasture grass is described as "leafy vegetation." However, the leafy vegetable group, as defined in Section 5.3.1.1, is composed of bulkier produce such as broccoli, brussel sprouts, cauliflower, celery, lettuce, and spinach. In addition, the outer leaves of most of the produce in this category are removed during preparation. Therefore, the VG_{ag} value of 1.0 for leafy vegetables is inappropriate and may overestimate COPC concentrations. A default lipophilic COPC VG_{ag} value of 0.01 for leafy vegetables is more appropriate for leafy vegetables because the leafy vegetable category represents bulkier, more protected plants as compared to single leaves of grass blades. U.S. EPA (1994r) and NC DEHNR (1997) recommend a lipophilic COPC VG_{ag} value of 0.01, for all classes of aboveground produce.

U.S. EPA OSW recommends using a lipophilic COPC (log K_{ow} greater than 4) VG_{ag} value of 0.01 for all aboveground exposed produce. For COPCs with a log K_{ow} less than 4, U.S. EPA OSW recommends using a VG_{ag} value of 1.0, because these COPCs are assumed pass more easily through the skin of produce.

Recommended Values for:
Empirical Correction Factor for Aboveground Produce (VG_{ag})

0.01 for COPCs with a log K_{ow} greater than 4

1.0 for COPCs with a log K_{ow} less than 4

Uncertainty may be introduced by the assumption of VG_{ag} values for leafy vegetables (such as lettuce) and for legumes (such as snap beans). Underestimation may be introduced by assuming a VG_{ag} value of 0.01 for legumes and leafy vegetables because these species often have a higher ratio of surface area to mass than other bulkier fruits and fruiting vegetables, such as tomatoes.

5.3.3 Produce Concentration Due to Root Uptake (*Pr*)
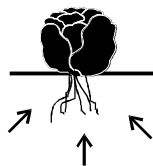
 Root uptake of contaminants from soil may also result in COPC concentrations in aboveground exposed produce, aboveground protected produce, and belowground produce. Consistent with previous guidance (U.S. EPA 1994m; U.S. EPA 1994r; and U.S. EPA 1995e), U.S. EPA OSW recommends the use of Equations 5-20A and 5-20B to calculate COPC

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concentration aboveground and belowground produce due to root uptake (*Pr*). The use of this equation is further described in Appendix B.

Recommended Equation for Calculating:
Produce Concentration Due to Root Uptake (*Pr*)

Exposed and protected aboveground produce:

$$Pr = Cs \cdot Br$$

Equation 5-20A

Belowground produce:

$$Pr = \frac{Cs \cdot RCF \cdot VG_{rootveg}}{Kd_s \cdot 1 \ kg/L}$$

Equation 5-20B

---

where

Pr	=	Concentration of COPC in produce due to root uptake (mg/kg)
Br	=	Plant-soil bioconcentration factor for produce (unitless)
$VG_{rootveg}$	=	Empirical correction factor for belowground produce (unitless)
Kd_s	=	Soil-water partition coefficient (L/kg)
Cs	=	Average soil concentration over exposure duration (mg COPC/kg soil)
RCF	=	Root concentration factor (unitless)

Equation 5-20A is based on the soil-to-aboveground plant transfer approach developed by Travis and Arms (1988). This approach is appropriate for evaluation of exposed and protected aboveground produce; however, it may not be appropriate for soil-to-belowground plant transfers. For belowground produce, U.S. EPA (1994m) and U.S. EPA (1995e) presented Equation 5-20B which includes a root concentration factor (RCF) developed by Briggs et al. (1982). RCF is the ratio of COPC concentration in the edible root to the COPC concentration in the soil water. Since Briggs et al. (1982) conducted their

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experiments in a growth solution, the COPC soil concentration (*Cs*) must be divided by the COPC-specific soil-water partition coefficient (*Kd$_s$*) (U.S. EPA 1994m).

Appendix A-3 describes determination of compound specific parameters *Br*, *Kd$_s$*, and *RCF*. Appendix B and Section 5.2 describe calculation of *Cs*. Similar to *VG$_{ag}$* and as discussed in Section 5.3.2.1, *VG$_{rootveg}$* is based on the lipophilicity of the COPC. Consistent with U.S. EPA (1994m), U.S. EPA OSW recommends a value of 0.01 for lipophilic COPCs (log K$_{ow}$ greater than 4) based on root vegetables like carrots and potatoes, because it appears to be the most complete and thorough information available. For COPCs with a log K$_{ow}$ less than 4, U.S. EPA OSW recommends a *VG$_{rootveg}$* value of 1.0.

Recommended Values for:
Empirical Correction Factor for Belowground Produce (*VG$_{rootveg}$*)

0.01 for COPCs with a log K$_{ow}$ greater than 4

1.0 for COPCs with a log K$_{ow}$ less than 4

5.4   CALCULATION OF COPC CONCENTRATIONS IN BEEF AND DAIRY PRODUCTS

COPC concentrations in beef tissue and milk products are estimated on the basis of the amount of COPCs that cattle are assumed to consume through their diet. The cattle's diet is assumed to consist of:

(1)   forage (primarily pasture grass and hay),

(2)   silage (forage that has been stored and fermented), and

(3)   grain.

Additional contamination may occur through the cattle's ingestion of soil. The total COPC concentration in the feed items (e.g., forage, silage, and grain) is calculated as a sum of contamination occurring through the following mechanisms:

*   **Direct deposition of particles**—wet and dry deposition of particle phase COPCs onto forage and silage (Section 5.4.1).

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- **Vapor transfer**—uptake of vapor phase COPCs by forage and silage through foliage (Section 5.4.2).

- **Root uptake**—root uptake of COPCs available from the soil and their transfer to the aboveground portions of forage, silage, and grain (Section 5.4.3).

Feed items consumed by animals can be classified as exposed and protected, depending on whether it has a protective outer covering. Because the outer covering on the protected feed acts as a barrier, it is assumed that there is negligible contamination of protected feed through deposition of particles and vapor transfer. In this analysis, grain is classified as protected feed. As a result, grain contamination is assumed to occur only through root uptake. Contamination of exposed feed items, including forage and silage, is assumed to occur through all three mechanisms.
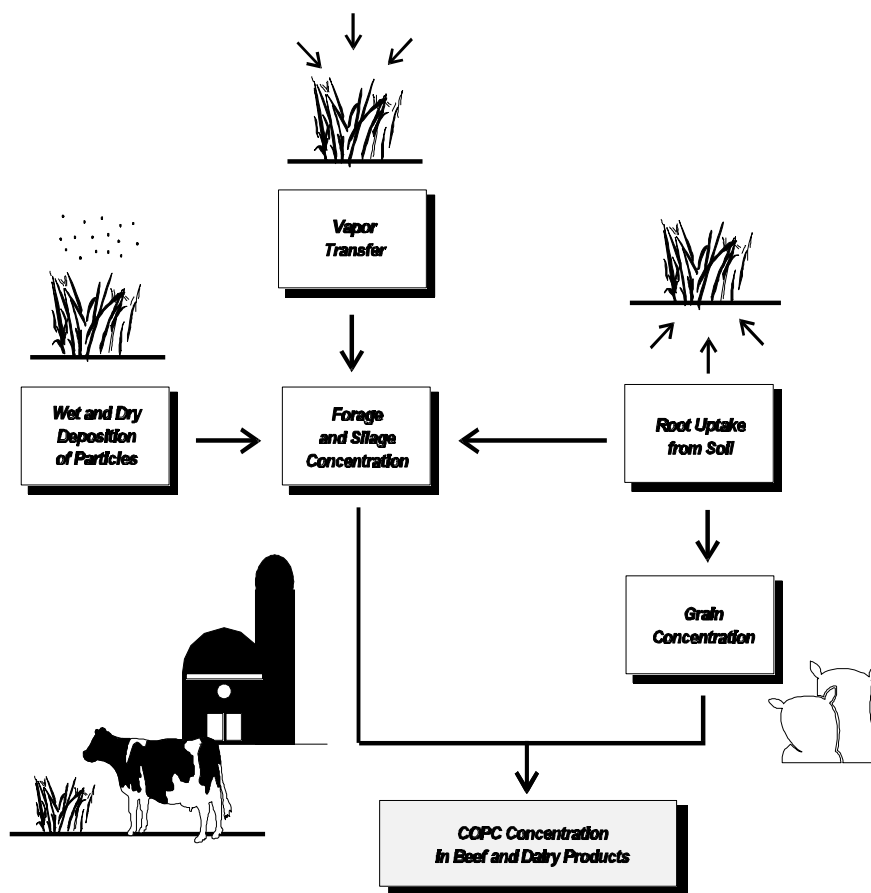
Figure 5-4 - COPC Concentration in Beef and Dairy Products

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The amount of grain, silage, forage, and soil consumed is assumed to vary between dairy and beef cattle. Sections 5.4.4 (beef) and 5.4.5 (dairy) describe methods for estimating consumption rates and subsequent COPC concentrations in cattle. Consistent with previous guidance (U.S. EPA 1990e; U.S. EPA 1994a; NC DEHNR 1997), U.S. EPA OSW recommends that 100 percent of the plant materials eaten by cattle be assumed to have been grown on soil contaminated by emission sources. Therefore, 100 percent of the feed items consumed are assumed to be contaminated.

Appendix B, Tables B-3-1 through B-3-11, describe calculation of (1) the COPC concentrations in soil and feed items (forage, silage, and grain) consumed by beef and dairy cattle, and (2) the resulting COPC concentrations in beef and milk.

5.4.1   Forage and Silage Concentrations Due to Direct Deposition (*Pd)*

COPC concentrations in forage and silage result from wet and dry deposition onto exposed plant surfaces; similar to aboveground produce (Section 5.3.1). Equation 5-14, described in Section 5.3.1, is recommended for calculation of COPC concentrations resulting from direct deposition onto plant surfaces of leafy plants and exposed produce (*Pd*). Therefore, U.S. EPA OSW recommends that Equation 5-14 also be used in calculating forage and silage concentrations due to direct deposition. Appendix B further describes calculation of COPC concentrations in forage and silage. Appendix A-3 describes determination of compound specific parameters *Fv*, *Bv*, and *Br*, which are calculated for forage and silage exactly as they are calculated for aboveground produce. *Rp*, *kp*, *Tp*, and *Yp* for use in calculating forage and silage concentrations are described in Sections 5.4.1.1 through 5.4.1.4.

5.4.1.1 Interception Fraction of the Edible Portion of Plant (*Rp*)

As discussed in Section 5.3.1.1, Chamberlain (1970) found a correlation between *Rp* and productivity, *Yp* (standing crop biomass). This correlation is expressed in Equation 5-14A.

Based on U.S. EPA (1994r), U.S. EPA (1995b) and NC DEHNR (1997), U.S. EPA OSW recommends that Equation 5-14 be used to calculate *Rp* values for forage and silage.

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Substituting the Baes, Sharp, Sjoreen, and Shor (1984) empirical constant (γ) value of 2.88 for pasture grass, and the standing crop biomass value of 0.24 kg DW/m^2 (these variables are discussed in Section 5.3.1.1) into Equation 5-14, the forage Rp is calculated to be 0.5. Substituting the Baes, Sharp, Sjoreen, and Shor (1984) empirical constant (γ) value of 0.769 for silage, and the standing crop biomass value of 0.8 kg DW/m^2 into Equation 5-14, the silage Rp value is calculated to be 0.46.

Recommended Value for:
Interception Fraction of the Edible Portion of Plant (Rp)

Forage = 0.5
Silage = 0.46

Several uncertainties are associated with the Rp variable:

(1) The empirical relationship developed by Chamberlain (1970) is based on a study of pasture grass and, therefore, may not accurately represent site-specific silage types.

(2) The empirical constant for silage developed by Baes, Sharp, Sjoreen, and Shor (1984) for use in Chamberlain's empirical relationship may also fail to accurately represent site-specific silage types.

(3) The range of empirical constants recommended by Baes, Sharp, Sjoreen, and Shor (1984) for pasture grass does not result in a significant range of estimated Rp values for forage (the calculated Rp range is 0.42 to 0.54).

Therefore, the use of the empirical constant midpoint (2.88 for pasture grass) does not significantly affect the Rp value and the resulting estimate of plant COPC concentration.

5.4.1.2 Plant Surface Loss Coefficient (kp)

Equation 5-15 (Section 5.3.1.2) presents the calculation of the plant surface loss coefficient kp for aboveground produce. The kp factor is derived in exactly the same manner for cattle forage and silage, and the uncertainties of kp for cattle forage and silage are similar to its uncertainties for aboveground produce.

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5.4.1.3 Length of Plant Exposure to Deposition per Harvest of the Edible Portion of Plant (*Tp*)

As discussed in Section 5.3.1.3, *Tp* is treated as a constant, based on the average period between successive hay harvests. This period, which was estimated at 60 days by Belcher and Travis (1989), represents the length of time that aboveground vegetation (in this case, hay) would be exposed to particle deposition before being harvested. Using Equation 5-16 (Section 5.3.1.3), *Tp* is calculated to be 0.16 year for cattle silage.

For cattle forage, Equation 5-16 is modified to consider the average of :

      (1)   the average period between successive hay harvests, and

      (2)   the average period between successive grazing.

Based on Belcher and Travis (1989), the average period between hay harvests is assumed to be 60 days, and the average period between successive grazing is assumed to be 30 days. *Tp* is therefore calculated as follows:

$$Tp = \frac{0.5 \cdot (60 \; days \; + \; 30 \; days)}{365 \; days/yr} = 0.12 \; yr \qquad \text{Equation 5-21}$$

Recommended Value for:
Plant Exposure Length to Deposition per Harvest of the Edible Portion of Plant (*Tp*)
Forage = 0.12 yr Silage = 0.16 yr

The primary uncertainties associated with *Tp* are similar to those for aboveground produce, and are discussed in Section 5.3.1.3.

5.4.1.4 Standing Crop Biomass (Productivity) (*Yp*)

As discussed in Section 5.3.1.4, U.S. EPA (1990e) stated that the best estimate of *Yp* is productivity, which is defined in Equation 5-17. This definition of *Yp* requires consideration of dry harvest yield (*Yh*) and area harvested (*Ah*).

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U.S. EPA OSW recommends that forage Yp be calculated as a weighted average of the calculated pasture grass and hay Yp values. Weightings are assumed to be 0.75 for forage and 0.25 for hay, based on the fraction of a year that cattle are assumed to be pastured and eating grass (9 months per year) or not pastured and fed hay (3 months per year). An unweighted pasture grass Yp of 0.15 kg DW/m^2 is assumed (U.S. EPA 1994r; U.S. EPA 1994m). An unweighted hay Yp of 0.5 kg DW/m^2 is calculated by using Equation 5-17 and the following Yh and Ah values:

- Yh = 1.22×10^{11} kg DW, calculated from the 1993 U.S. average wet weight Yh of 1.35×10^{11} kg (USDA 1994b) and a conversion factor of 0.9 (Fries 1994).

- Ah = 2.45×10^{11} m^2, the 1993 U.S. average for hay (USDA 1994b).

The unweighted pasture grass and hay Yp values are multiplied by their weighting factors (0.75 and 0.25, respectively), and then added to calculate the weighted forage Yp of 0.24 kg DW/m^2.

U.S. EPA OSW recommends that a production-weighted U.S. average Yp of 0.8 kg DW/m^2 be assumed for silage (Shor, Baes, and Sharp 1982).

Recommended Values for:
Standing Crop Biomass (Productivity) (Yp)

Forage = 0.24 kg DW/m^2
Silage = 0.8 kg DW/m^2

The primary uncertainty associated with this variable is that the harvest yield (Yh) and area planted (Ah) may not reflect site-specific conditions. To the extent that site-specific information is available, the magnitude of the uncertainty introduced by the default Yp value can be estimated. In addition, the weightings assumed in this discussion for the amount of time that cattle are pastured (and foraging) or stabled (and being fed silage) should be adjusted to reflect site-specific conditions, as appropriate.

5.4.2   Forage and Silage Concentrations Due to Air-to-Plant Transfer (Pv)

COPC concentration in aboveground produce resulting from air-to-plant transfer (Pv), is calculated by using Equation 5-18 (Section 5.3.2). Pv is calculated for cattle forage and silage similarly to the way that it is calculated for aboveground produce. A detailed discussion of Pv is provided in Section 5.3.2.

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Differences in VG_{ag} values for forage and silage, as compared to the values for aboveground produce described in Section 5.3.2.1, are presented below in Section 5.4.2.1. The calculation of Pv is further described in Appendix B.

5.4.2.1 Empirical Correction Factor for Forage and Silage (VG_{ag})

U.S. EPA (1994m) recommended a VG_{ag} of 1.0 for pasture grass and other leafy vegetation because of a direct analogy to exposed azalea and grass leaves. Pasture grass is described as "leafy vegetation." U.S. EPA (1994m) and NC DEHNR (1997) recommended a VG_{ag} to reduce estimated concentrations of COPCs in specified types of vegetation. Such a factor can be used to reduce estimated silage concentrations if it is assumed that there is insignificant translocation of COPCs deposited on the surface of bulky silage to the inner parts of the vegetation. Application of a silage VG_{ag} would be relevant if the silage cannot be characterized as leafy (e.g., if grain is used as silage). As a point of clarification, forage and silage are considered vegetative plant parts, and grains are considered reproductive plant parts.

U.S. EPA (1994m) did not recommend a VG_{ag} value for silage. NC DEHNR (1997) recommended a VG_{ag} factor of 0.5 for bulky silage but does not present a specific rationale for this value. U.S. EPA (1995b) noted that a volume ratio of outer whole surface area to volume of vegetation could be used to assign a silage VG_{ag} value, if specific assumptions—concerning the proportions of each type of vegetation of which silage may consist—were known. However, in the absence of specific assumptions concerning the quantities of different silage material (e.g., hay and grain), U.S. EPA (1995b) recommended assuming a VG_{ag} of 0.5 for silage without rigorous justification.

U.S. EPA OSW recommends the use of VG_{ag} values of 1.0 for forage and 0.5 for silage. As discussed, the primary uncertainty associated with this variable is the lack of specific information on the proportions of each vegetation type of which silage may consist, leading to the default assumption of 0.5.

Recommended Values for: **Empirical Correction Factor for Forage and Silage (VG_{ag})**
Forage = 1 Silage = 0.5

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5.4.3   Forage, Silage, and Grain Concentrations Due to Root Uptake (*Pr*)
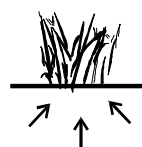
COPC concentration in aboveground and belowground produce resulting from root uptake is calculated by using Equations 5-20A and 5-20B (Section 5.3.3). *Pr* is also calculated for cattle forage, silage, and grain in exactly the same way that it is calculated for aboveground produce. A detailed discussion describing calculation of *Pr* is provided in Section 5.3.3.

The calculation of *Pr* is further described in Appendix B.

5.4.4   Beef Concentration Resulting from Plant and Soil Ingestion (A_{beef})

Consistent with U.S. EPA (1995h), U.S. EPA OSW recommends that COPC concentration in beef tissue (A_{beef}) be calculated by using Equation 5-22. The equation was modified from an equation presented in U.S. EPA (1990c), U.S. EPA (1994r), U.S. EPA (1995b), and NC DEHNR (1996) by the introduction of a metabolism factor (MF). Equation 5-22 calculates the daily amount of a COPC that is consumed by cattle through the ingestion of contaminated feed items (plant) and soil. The equation includes biotransfer and metabolism factors to transform the daily animal intake of a COPC (mg/day) into an animal COPC tissue concentration (mg COPC/kg tissue). The use of this equation is further described in Appendix B, Table 3-10.

Recommended Equation for Calculating:
Concentration of COPC in Beef (A_{beef})

$$A_{beef} = \left(\sum (F_i \cdot Qp_i \cdot P_i) + Qs \cdot Cs \cdot Bs \right) \cdot Ba_{beef} \cdot MF \qquad \text{Equation 5-22}$$

---

where

A_{beef}	=	Concentration of COPC in beef (mg COPC/kg FW tissue)
F_i	=	Fraction of plant type i grown on contaminated soil and ingested by the animal (cattle) (unitless)
Qp_i	=	Quantity of plant type i eaten by the animal (cattle) per day (kg DW plant/day)
P_i	=	Concentration of COPC in each plant type i eaten by the animal (cattle) (mg/kg DW)

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Qs	=	Quantity of soil eaten by the animal (cattle) each day (kg/day)
Cs	=	Average soil concentration over exposure duration (mg COPC/kg soil)
Bs	=	Soil bioavailability factor (unitless)
Ba_{beef}	=	COPC biotransfer factor for beef (day/kg FW tissue)
MF	=	Metabolism factor (unitless)

Appendix A-3 describes determination of the compound specific parameter Ba_{beef}. The parameters F_i, Qp_i, P_i, Qs, Cs, Bs, and MF are described in Sections 5.4.4.1 through 5.4.4.7, respectively.

5.4.4.1 Fraction of Plant Type i Grown on Contaminated Soil and Eaten by the Animal (Cattle)(F_i)

Consistent with U.S. EPA (1990e), U.S. EPA (1994r), and NC DEHNR (1997), U.S. EPA OSW recommends that 100 percent of the plant materials eaten by cattle be assumed to have been grown on soil contaminated by the emission sources being evaluated. U.S EPA OSW recommends a default value of 1.0 for F_i.

Recommended Value for:

Fraction of Plant Type i Grown on Contaminated Soil and Eaten by the Animal (Cattle) (F_i)

1

5.4.4.2 Quantity of Plant Type i Eaten by the Animal (Cattle) Each Day (Qp_i)

The daily quantity of plants eaten by cattle should be estimated (kg DW/day) for each category of plant feed. Forage, silage, and grain feeds should be included in this estimate (U.S. EPA 1990e; U.S. EPA 1994r; NC DEHNR 1997).

NC DEHNR (1997) recommended plant ingestion rates for the cattle of either subsistence beef farmers or typical beef farmers. Subsistence beef farmers rely on a higher percentage of forage and silage to feed cattle, whereas typical beef farmers rely on greater amounts of grain to feed cattle. U.S. EPA (1990e) and U.S. EPA (1994r) identified plant ingestion rates only for subsistence farmers. The following daily quantity of forage, grain, and silage eaten by cattle was recommended by NC DEHNR (1997), U.S. EPA (1994r), U.S. EPA (1990e), and Boone, Ng, and Palm (1981):

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Source	Forage (kg DW/day)	Grain (kg DW/day)	Silage (kg DW/day)	References
NC DEHNR (1997) Subsistence Farmer Beef Cattle	8.8	0.47	2.5	Boone, Ng, and Palm (1981) NAS (1987)
NC DEHNR (1997) Typical Farmer Beef Cattle	3.8	3.8	1.0	Rice (1994)
U.S. EPA (1994r) Subsistence Farmer Beef Cattle	8.8	Not reported	Not reported	Boone, Ng, and Palm (1981) NAS (1987)
U.S. EPA (1990e) Subsistence Farmer Beef Cattle	8.8	0.47	2.5	Boone, Ng, and Palm (1981) McKone and Ryan (1989)
Boone, Ng, and Palm (1981)	8.87	1.9	2.5	Boone, Ng, and Palm (1981)

With the exception of a higher grain ingestion rate, Boone, Ng, and Palm (1981) rates are consistent with those recommended by U.S. EPA (1990e), U.S. EPA (1994r), and NC DEHNR (1997). For typical farmer beef cattle, NC DEHNR (1997) cites Rice (1994) as a reference for the Qp_i variables and notes that the values include grain supplemented during the growing phase for beef cattle.

U.S. EPA (1990e) noted that McKone and Ryan (1989) reported an average total ingestion rate of 12 kg DW/day for the three plant feeds, which is consistent with the total recommended by U.S. EPA (1990e) and NC DEHNR (1997) (forage, grain, and silage total of 11.8 kg DW/day). U.S. EPA (1994r) and NC DEHNR (1997) also noted that NAS (1987) reported a daily dry matter intake that is 2 percent of an average beef cattle body weight of 590 kilograms. This results in a daily total intake rate of 11.8 kg DW/day. NAS (1987) reported that a nonlactating cow eats dry matter equivalent to 2 percent of its body weight.

U.S. EPA OSW recommends the following beef cattle ingestion rates of forage, silage, and grain. These values are based on the total daily intake rate of about 12 kg DW/day.

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Recommended Values for:
Quantity of Plant Type i Eaten by the Animal (Cattle) Each Day (Qp_i)

Forage = 8.8 kg DW/day
Silage = 2.5 kg DW/day
Grain = 0.47 kg DW/day

The principal uncertainty associated with Qp_i is the variability between forage, silage, and grain ingestion rates for cattle.

5.4.4.3 Concentration of COPC in Plant Type i Eaten by the Animal (Cattle) (P_i)

The total COPC concentration in forage, silage, and grain should be calculated by using Equation 5-23. Values for Pd, Pv, and Pr should be derived for each type of feed by using Equations 5-14, 5-18, and 5-20, respectively.

Recommended Equation for Calculating:
Concentration of COPC in Plant Type i Eaten by the Animal (Cattle) (P_i)

$$P_i = \sum_i (Pd + Pv + Pr) \qquad\qquad \text{Equation 5-23}$$

where

P_i	=	Concentration of COPC in each plant type i eaten by the animal (mg COPC/kg DW)
Pd	=	Plant concentration due to direct deposition (mg COPC/kg DW)
Pv	=	Plant concentration due to air-to-plant transfer (mg COPC/kg DW)
Pr	=	Plant concentration due to root uptake (mg COPC/kg DW)

This equation is further described in Appendix B.

5.4.4.4 Quantity of Soil Eaten by the Animal (Cattle) Per Day (Qs)

Additional cattle contamination occurs through ingestion of soil. U.S. EPA OSW recommends a value of 0.5 kg/day for the quantity of soil ingested by the animal (cattle).

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Recommended Value for:
Quantity of Soil Ingested by the Animal (Cattle) Per Day (Qs)

0.5 kg/day

NC DEHNR (1997) and U.S. EPA (1994r) recommended a soil ingestion rate for subsistence beef cattle of 0.5 kg/day. This rate is based on Fries (1994). U.S. EPA (1994r) and NC DEHNR (1997) noted that Fries (1994) reported soil ingestion to be 4 percent of the total dry matter intake. NAS (1987) was also referenced. NAS (1987) cited an average beef cattle weight of 590 kg, and a daily dry matter intake rate (nonlactating cows) of 2 percent of body weight. This results in a daily dry matter intake rate of 11.8 kg DW/day and a daily soil ingestion rate of about 0.5 kg/day. U.S. EPA (1990e) reported a soil ingestion rate that is 3 percent of the forage intake rate of 8.8 kg DW/day, resulting in a daily soil ingestion rate of approximately 0.3 kg/day. Simmonds and Linsley (1981) and Thornton and Abrams (1983) were cited as the references for this assumption.

5.4.4.5 Average Soil Concentration Over Exposure Duration (Cs)

COPC concentration in soil should be calculated as discussed in Section 5.2.1, by using Equations 5-1C, 5-1D, and 5-1E. Also, Appendix B further describes calculation of the soil concentration.

5.4.4.6 Soil Bioavailability Factor (Bs)

Soil bioavailability factor, Bs, is defined as the ratio between bioconcentration (or biotransfer) factors for soil and vegetation for a given COPC. The efficiency of transfer from soil may differ from efficiency or transfer from plant material for some COPCs. If the transfer efficiency is lower for soils, than this ratio would be less than 1.0. If it is equal or greater than that of vegetation, the Bs value would be equal to or greater than 1.0.

Until more COPC-specific data becomes available for this parameter, U.S. EPA OSW recommends a default value of 1 for Bs.

Recommended Values for:
Soil Bioavailability Factor (Bs)

1.0

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5.4.4.7 Metabolism Factor (*MF*)

The metabolism factor (*MF*) represents the estimated amount of COPC that remains in fat and muscle. Based on a study by Ikeda et al. (1980), U.S. EPA (1995h) utilized a COPC-specific *MF* to account for metabolism in animals and humans. Consistent with U.S. EPA (1995h), U.S. EPA recommends a *MF* of 0.01 for bis(2-ethylhexyl)phthalate (BEHP), and 1.0 for all other COPCs. Evidence indicates BEHP is more readily metabolized and excreted by mammalian species than other contaminants (ATSDR 1987). Considering the recommended values for this variable, *MF* has no quantitative effect on A_{beef} (with the exception of BEHP).

MF applies only to mammalian species, including beef cattle, dairy cattle, and pigs. It does not relate to metabolism in produce, chicken, or fish. In addition, since exposures evaluated in this guidance are intake driven, the use of a metabolism factor applies only to food sources used in evaluating indirect human exposure, including ingestion of beef, milk, and pork. In summary, use of a *MF* does not apply for direct exposures to air, soil, or water, or to ingestion of produce, chicken, or fish.

5.4.5   COPC Concentration In Milk Due to Plant and Soil Ingestion (A_{milk})

Equation 5-22 (Section 5.4.4) describes the calculation of COPC concentrations in beef cattle (A_{beef}). Equation 5-22 can be modified to calculate COPC milk concentrations (A_{milk}), as follows:

Recommended Equation for Calculating:
Concentration of COPC in Milk (A_{milk})

$$A_{milk} = \left(\sum (F_i \cdot Qp_i \cdot P_i) + Qs \cdot Cs \cdot Bs \right) \cdot Ba_{milk} \cdot MF \qquad \text{Equation 5-24}$$

---

where

A_{milk}	=	Concentration of COPC in milk (mg COPC/kg milk)
F_i	=	Fraction of plant type *i* grown on contaminated soil and ingested by the animal (dairy cattle) (unitless)

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Qp_i	=	Quantity of plant type i eaten by the animal (dairy cattle) each day (kg DW plant/day)
P_i	=	Concentration of COPC in plant type i eaten by the animal (dairy cattle) (mg/kg DW)
Qs	=	Quantity of soil eaten by the animal (dairy cattle) each day (kg soil/day)
Cs	=	Average soil concentration over exposure duration (mg COPC/kg soil)
Bs	=	Soil bioavailability factor (unitless)
Ba_{milk}	=	COPC biotransfer factor for milk (day/kg WW tissue)
MF	=	Metabolism factor (unitless)

U.S. EPA OSW recommends the use of Equation 5-24 to estimate dairy cattle milk COPC concentration (A_{milk}). Appendix A-3 describes determination of the compound specific parameter Ba_{milk}. The use of this equation is further described in Appendix B, Table B-3-11.

The discussion in Section 5.4.4 of the variables F_i, Qp_i, P_i, Qs, Cs, and MF for beef cattle generally applies to the corresponding variables for dairy cattle. However, there are some differences in assumptions made for dairy cattle; these differences are summarized in the following subsections.

5.4.5.1 Fraction of Plant Type i Grown on Contaminated Soil and Eaten by the Animal (Dairy Cattle) (F_i)

The calculation of F_i for dairy cattle is identical to that for beef cattle (Section 5.4.4.1).

5.4.5.2 Quantity of Plant Type i Eaten by the Animal (Dairy Cattle) Per Day (Qp_i)

As discussed in Section 5.4.4.2, the daily quantity of forage, silage, and grain feed consumed by cattle is estimated for each category of feed material. However, daily ingestion rates for dairy cattle are estimated differently than for beef cattle. The daily quantity of feed consumed by cattle should be estimated on a dry weight basis for each category of plant feed.

NC DEHNR (1997) recommended the use of plant ingestion rates for either subsistence dairy farmer or typical dairy farmer cattle. In addition, subsistence dairy farmers rely on a higher percentage of forage and silage to feed cattle, whereas typical dairy farmers rely on greater amounts of grain to feed cattle. U.S. EPA (1990e) and U.S. EPA (1994r) identified plant ingestion rates only for subsistence farmers.

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The following daily quantity of forage, grain, and silage eaten by dairy cattle was recommended by NC DEHNR (1997), U.S. EPA (1994r), U.S. EPA (1990e), and Boone, Ng, and Palm (1981):

Source	Forage (kg/day DW)	Grain (kg/day DW)	Silage (kg/day DW)	References
NC DEHNR (1997) Subsistence Dairy Farmer Cattle	13.2	3.0	4.1	Boone, Ng, and Palm (1981) NAS (1987)
NC DEHNR (1997) Typical Dairy Farmer Cattle	6.2	12.2	1.9	Rice (1994)
U.S. EPA (1994r) Subsistence Dairy Farmer Cattle	13.2	Not reported	Not reported	Boone, Ng, and Palm (1981) NAS (1987)
U.S. EPA (1990e) Subsistence Dairy Farmer Cattle	11.0	2.6	3.3	Boone, Ng, and Palm (1981) McKone and Ryan (1989)
Boone, Ng, and Palm (1981)	11.0	2.6	3.3	Boone, Ng, and Palm (1981)

U.S. EPA (1990e) notes that McKone and Ryan (1989) reports an average total ingestion rate of 17 kg/day DW for the three plant feeds, which is consistent with the total ingestion rate recommended by U.S. EPA (1990e). U.S. EPA (1994r) and NC DEHNR (1997) noted that NAS (1987) reports a daily dry matter intake that is 3.2 percent of an average dairy cattle body weight of 630 kilograms. This results in a daily total intake rate of approximately 20 kg/day DW, which is consistent with the average total ingestion rates for the three plant feeds recommended by U.S. EPA (1994r) and NC DEHNR (1997) . NAS (1987) reported that dairy cows eat dry matter equivalent to 3.2 percent of their body weight; the 630-kilogram average dairy cow body weight was not confirmed. U.S. EPA (1995b) also cited a feed ingestion rate of 20 kg/day DW, citing U.S. EPA (1993d).

Based on more recent references (NAS 1987; U.S. EPA 1993d) which recommend a feed ingestion rate of 20 kg/day DW, U.S. EPA OSW recommends a default total ingestion rate of 20 kg DW/day for dairy cattle.

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Recommended Values for:
Quantity of Plant Type *i* Eaten by the Animal (Dairy Cattle) Per Day (Qp_i)
Forage = 13.2 kg DW/day Silage = 4.1 kg DW/day Grain = 3.0 kg DW/day

Uncertainties associated with the estimation of Qp_i include the estimation of forage, grain, and silage
ingestion rates, which will vary from site to site. The assumption of uniform contamination of plant
materials consumed by cattle also introduces uncertainty.

5.4.5.3 Concentration of COPC in Plant Type *i* Eaten by the Animal (Dairy Cattle) (P_i)

The estimation of P_i for dairy cattle is identical to that for beef cattle (Section 5.4.4.3).

5.4.5.4 Quantity of Soil Eaten by the Animal (Dairy Cattle) Per Day (Qs)

As discussed in Section 5.4.4.4, contamination of dairy cattle also results from the ingestion of soil.
U.S. EPA OSW recommends the following soil ingestion rates for dairy cattle:

Recommended Values for:
Quantity of Soil Eaten by the Animal (Dairy Cattle) Per Day (Qs)
0.4 kg/day

U.S. EPA (1994r) and NC DEHNR (1997) recommended a soil ingestion rate of 0.4 kg/day for
subsistence farmer dairy cattle, based on Fries (1994). U.S. EPA (1994r) and NC DEHNR (1997) noted
that Fries (1994) reported soil ingestion rates as 2 percent of the total dry matter intake. NAS (1987) was
also referenced, which reported an average dairy cattle weight of 630 kilograms and a daily dry matter
intake rate (nonlactating cows) of 3.2 percent of body weight. This resulted in a daily dry matter intake
rate of 20 kg/day DW, and a daily soil ingestion rate of approximately 0.4 kg/day. NC DEHNR (1997)
recommended a soil ingestion rate of 0.2 kg/day for the cattle of typical dairy farmers, citing Rice (1994).

U.S. EPA (1990e) reported soil ingestion rates as 3 percent of the forage intake rate. It was assumed that
the more conservative forage intake rate of 13.2 kg/day DW results in a daily soil ingestion rate of about

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0.4 kg/day. Simmonds and Linsley (1981) and Thornton and Abrams (1983) were cited as the references for this assumption.

Uncertainties associated with *Qs* include the lack of current empirical data to support soil ingestion rates for dairy cattle. The assumption of uniform contamination of soil ingested by cattle also adds uncertainty.

5.4.5.5 Average Soil Concentration Over Exposure Duration (*Cs*)

The calculation of *Cs* for dairy cattle is the same as for beef cattle (Section 5.4.4.5).

5.4.5.6 Soil Bioavailability Factor (*Bs*)

The calculation of *Bs* for dairy cattle is the same as for beef cattle (Section 5.4.4.6).

5.4.5.7 Metabolism Factor (*MF*)

The recommended values for *MF* are identical to those recommended for beef cattle (Section 7.4.5.7).

5.5   CALCULATION OF COPC CONCENTRATIONS IN PORK

COPC concentrations in pork tissue are estimated on the basis of the amount of COPCs that swine are assumed to consume through their diet; assumed to consist of silage and grain. Additional COPC contamination of pork tissue may occur through the ingestion of soil by swine.

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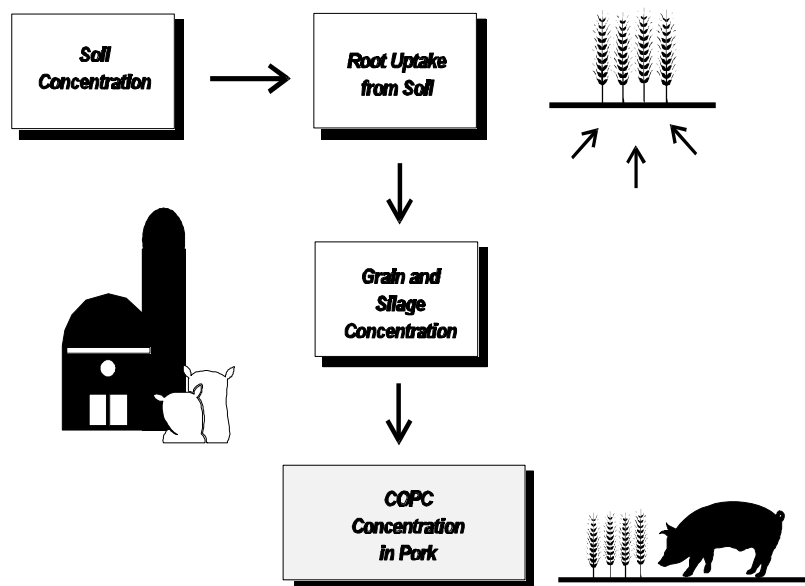
Figure 5-5 - COPC Concentration in Pork

5.5.1 Concentration of COPC In Pork

Equation 5-22 (Section 5.4.4) describes the calculation of COPC concentration in beef cattle (A_{beef}).
Equation 5-22 can be modified to calculate COPC concentrations in swine (A_{pork}), as follows:

Recommended Equation for Calculating:
Concentration of COPC in Pork (A_{pork})

$$A_{pork} = \left(\sum (F_i \cdot Qp_i \cdot P_i) + Qs \cdot Cs \cdot Bs \right) \cdot Ba_{pork} \cdot MF \qquad \text{Equation 5-25}$$

where

A_{pork}	=	Concentration of COPC in pork (mg COPC/kg FW tissue)
F_i	=	Fraction of plant type i grown on contaminated soil and ingested by the animal (swine)(unitless)
Qp_i	=	Quantity of plant type i eaten by the animal (swine) each day (kg DW plant/day)

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P_i	=	Concentration of COPC in plant type i eaten by the animal (swine) (mg/kg DW)
Qs	=	Quantity of soil eaten by the animal (swine) (kg/day)
Cs	=	Average soil concentration over exposure duration (mg COPC/kg soil)
Bs	=	Soil bioavailability factor (unitless)
Ba_{pork}	=	COPC biotransfer factor for pork (day/kg FW tissue)
MF	=	Metabolism factor (unitless)

U.S. EPA OSW recommends that Equation 5-25 be used to calculate COPC pork concentrations (A_{pork}). Appendix A-3 describes determination of the compound specific parameter Ba_{pork}. This equation is further described in Appendix B, Table B-3-12. The discussion in Section 5.4.5 of the variables F_i, Qp_i, P_i, Qs, Cs and MF for beef cattle generally applies to the corresponding variables for pork. However, different assumptions are made for pork. These differences are summarized in the following subsections.

5.5.1.1 Fraction of Plant Type i Grown on Contaminated Soil and Eaten by the Animal (Swine) (F_i)

The calculation of F_i for pork is identical to that for beef cattle (Section 5.4.4.1).

5.5.1.2 Quantity of Plant Type i Eaten by the Animal (Swine) Each Day (Qp_i)

As discussed in Section 5.4.4.2, the daily quantity of forage, silage, and grain feed consumed by beef cattle is estimated for each category of feed material. However, daily ingestion rates for pork are estimated differently than for beef cattle. U.S. EPA (1990e), U.S. EPA (1994r), and NC DEHNR (1997) recommended that only silage and grain feeds be included in estimates of daily plant quantity eaten by swine. Because swine are not grazing animals, they are assumed not to eat forage (U.S. EPA 1990e). The daily quantity of plant feeds (kilograms of DW) consumed by swine should be estimated for each category of plant feed.

U.S. EPA (1990e) and NC DEHNR (1997) did not differentiate between subsistence and typical hog farmers as for cattle. U.S. EPA (1990e) and NC DEHNR (1997) recommended grain and silage ingestion rates for swine as 3.0 and 1.3 kg DW/day, respectively. NC DEHNR (1997) references U.S. EPA (1990e) as the source of these ingestion rates. U.S. EPA (1990e) reported total dry matter ingestion rates for hogs and lactating sows as 3.4 and 5.2 kg DW/day, respectively. U.S. EPA (1990e) cites Boone, Ng, and Palm (1981) as the source of the ingestion rate for hogs, and NAS (1987) as the source of the ingestion rate for a lactating sow. Boone, Ng, and Palm (1981) reported a grain ingestion rate of

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3.4 kg DW/day for a hog. NAS (1987) reported an average ingestion rate of 5.2 kg DW/day for a lactating sow. U.S. EPA (1990e) recommended using the average of these two rates (4.3 kg DW/day). U.S. EPA (1990e) assumed that 70 percent of the swine diet is grain and 30 percent silage to obtain the grain ingestion rate of 3.0 kg DW/day and the silage ingestion rate of 1.3 kg DW/day. U.S. EPA (1990e) cited U.S. EPA (1982b) as the source of the grain and silage dietary fractions. U.S. EPA (1995b) recommended an ingestion rate of 4.7 kg DW/day for a swine, referencing NAS (1987). NAS (1987) reported an average daily intake of 4.36 kg DW/day for a gilt (young sow) and a average daily intake of 5.17 kg DW/day for a sow, which averages out to 4.7 kg/DW/day. Assuming the 70 percent grain to 30 percent silage diet noted above, estimated ingestion rates of 3.3 kg DW/day (grain) and 1.4 kg DW/day (silage) are derived.

U.S. EPA OSW recommends the use of the more conservative ingestion rates. These rates are presented below:

Recommended Values for:
Quantity of Plant Type *i* Eaten by the Animal (Swine) Each Day (Qp_i)
Grain = 3.3 kg DW/day Silage = 1.4 kg DW/day

Uncertainties associated with this variable include the variability of actual grain and silage ingestion rates from site to site. Site-specific data can be used to mitigate this uncertainty. In addition, the assumption of uniform contamination of plant materials consumed by swine produces some uncertainty.

5.5.1.3 Concentration of COPC in Plant Type *i* Eaten by the Animal (Swine) (P_i)

The calculation of P_i for pork is identical to that for beef cattle (Section 5.4.4.3).

5.5.1.4 Quantity of Soil Eaten by the Animal (Swine) Each Day (Q_s)

As discussed in Section 5.4.4.4, additional contamination of swine results from ingestion of soil. The following Q_s values were recommended by U.S. EPA (1990e) and NC DEHNR (1997):

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Guidance	Quantity of Soil Eaten by Swine Each Day (Q_s)
U.S. EPA (1990e)	Stated that sufficient data are not available to estimate swine soil ingestion rates.
NC DEHNR (1997)	0.37 kg/day Estimated by assuming a soil intake that is 8% of the plant ingestion rate of 4.3 kg DW/day). U.S. EPA (1993h) was cited as the reference for the soil ingestion rate of 8 percent of dry matter intake.

Consistent with NC DEHNR (1997), U.S. EPA OSW recommends the following soil ingestion rate for swine:

Recommended Value for:
Quantity of Soil Eaten by the Animal (Swine) Each Day (Q_s)

0.37 kg DW/day

Uncertainties associated with this variable include the lack of current empirical data to support soil ingestion rates for swine, and the assumption of uniform contamination of soil ingested by swine.

5.5.1.5 Average Soil Concentration Over Exposure Duration (Cs)

The calculation of Cs for pork is the same as for beef cattle (Section 5.4.4.5).

5.5.1.6 Soil Bioavailability Factor (Bs)

The calculation of Bs for pork is the same as for beef cattle (Section 5.4.4.6)

5.5.1.7 Metabolism Factor (MF)

The recommended values for MF are identical to those recommended for beef cattle (Section 5.4.4.7).

5.6   CALCULATION OF COPC CONCENTRATIONS IN CHICKEN AND EGGS

Estimates of the COPC concentrations in chicken and eggs are based on the amount of COPCs that chickens consume through ingestion of grain and soil. The uptake of COPCs

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via inhalation and via ingestion of water is assumed to be insignificant. Chickens are assumed to be

free-range animals that have contact with soil; and therefore, are assumed to consume 10 percent of their

diet as soil, a percentage that is consistent with the study from which the biotransfer factors were

obtained (Stephens, Petreas, and Hayward 1995). The remainder of the diet (90 percent) is assumed to

consist of grain. Grain ingested by chickens is assumed to have originated from the exposure scenario

location; therefore, 100 percent of the grain consumed is assumed to be contaminated.
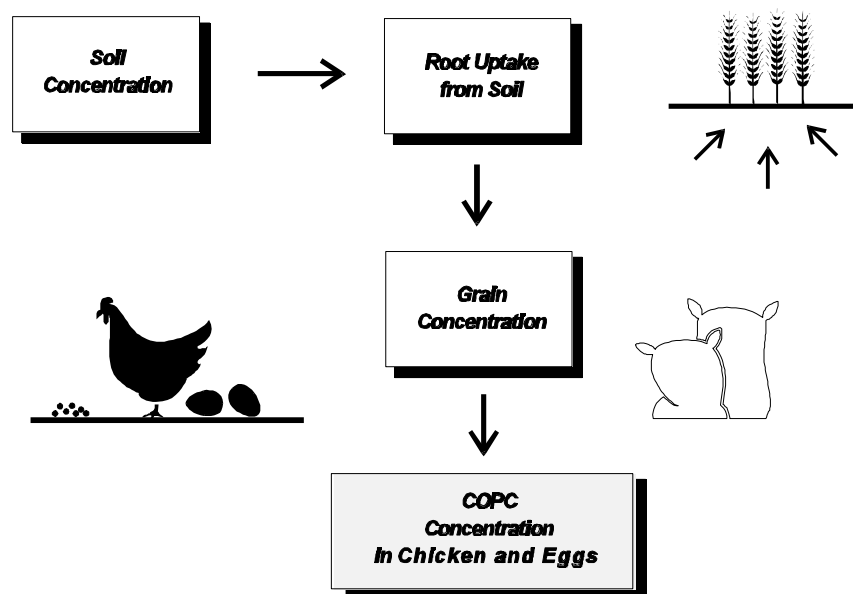
Figure 5-6 - COPC Concentration in Chicken and Eggs

The COPC concentration in grain is estimated by using the algorithm for aboveground produce described

in Section 5.3. Grain is considered to be a feed item that is protected from deposition of particles and

vapor transfer. As a result, only contamination due to root uptake of COPCs is considered in the

calculation of COPC concentration in grain. Equations for calculating concentrations in chicken and

eggs are presented in Appendix B. The methodology used to derive biotransfer factors and the

COPC-specific values for chicken and eggs are presented in Appendix A-3.

5.6.1 Concentration of COPC in Chicken and Eggs

Consistent with NC DEHNR (1997), U.S. EPA OSW recommends the use of Equation 5-26 to calculate

COPC concentrations in chicken and eggs (Stephens, Petreas, and Hayword 1995). COPC

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concentrations in chicken and eggs should be determined separately. Parameters and variables in

Equation 5-26 are further described in Appendix B, Tables B-3-13 and B-3-14.

Recommended Equation for Calculating:
Concentration of COPC in Chicken and Eggs ($A_{chicken}$ or A_{egg})

$$A_{chicken} \ or \ A_{egg} = (\Sigma[F_i \cdot Qp_i \cdot Pi] \ + \ Qs \cdot Cs \cdot Bs) \cdot (Ba_{egg} \ or \ Ba_{chicken})$$ Equation 5-26

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where

$A_{chicken}$	=	Concentration of COPC in chicken (mg COPC/kg FW tissue)
A_{egg}	=	Concentration of COPC in eggs (mg COPC/kg FW tissue)
F_i	=	Fraction of plant type i (grain) grown on contaminated soil and ingested by the animal (chicken)(unitless)
Qp_i	=	Quantity of plant type i (grain) eaten by the animal (chicken) each day (kg DW plant/day)
P_i	=	Concentration of COPC in plant type i (grain) eaten by the animal (chicken) (mg/kg DW)
Qs	=	Quantity of soil eaten by the animal (chicken) (kg/day)
Cs	=	Average soil concentration over exposure duration (mg COPC/kg soil)
Bs	=	Soil bioavailability factor (unitless)
$Ba_{chicken}$	=	COPC biotransfer factor for chicken (day/kg FW tissue)
Ba_{egg}	=	COPC biotransfer factor for eggs (day/kg FW tissue)

Appendix A-3 describes determination of compound specific parameters $Ba_{chicken}$ and Ba_{egg}. The

remaining parameters are discussed in Appendix B and in the following subsections.

5.6.1.1 Fraction of Plant Type i Grown on Contaminated Soil and Eaten by the Animal (Chicken)(F_i)

The calculation of F_i for chicken is identical to that for beef cattle (Section 5.4.4.1).

5.6.1.2 Quantity of Plant Type i Eaten by the Animal (Chicken) Each Day (Qp_i)

As discussed in Section 5.4.4.2, the daily quantity of forage, silage, and grain feed consumed by beef

cattle is estimated for each category of feed material. However, daily ingestion rates for chicken are

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estimated differently than for beef cattle. NC DEHNR (1997) recommended that only grain feeds be included in this estimate. Because chickens are not grazing animals, they are assumed not to eat forage (U.S. EPA 1990e). Chickens are assumed not to consume any silage. The daily quantity of plant feeds (kilograms of DW) consumed by chicken only should be estimated for grain feed.

Consistent with Ensminger (1980), Fries (1982), and NAS (1987), U.S. EPA OSW recommends the use of the following ingestion rate:

Recommended Value for:
Quantity of Plant Type i Eaten by the Animal (Chicken) Each Day (Qp_i)

Grain = 0.2 kg DW/day

Uncertainties associated with this variable include the variability of actual grain ingestion rates from site to site. In addition, the assumption of uniform contamination of plant materials consumed by chicken produces some uncertainty.

5.6.1.3 Concentration of COPC in Plant Type i Eaten by the Animal (Chicken) (P_i)

The total COPC concentration is the COPC concentration in grain and should be calculated by using Equation 5-27. Values for Pr should be derived by using Equation 5-20.

Recommended Equation for Calculating:
Concentration of COPC in Plant Type i Eaten by the Animal (Chicken) (P_i)

$$P_i = \sum_i (Pr)$$

Equation 5-27

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where

P_i = Concentration of COPC in each plant type i eaten by the animal (mg COPC/kg DW)

Pr = Plant concentration due to root uptake (mg COPC/kg DW)

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This equation is further described in Appendix B.

5.6.1.4 Quantity of Soil Eaten by the Animal (Chicken) Each Day (Qs)

COPC concentration in chickens also results from intake of soil. As discussed earlier, chickens are assumed to consume 10 percent of their total diet as soil, a percentage that is consistent with the study from Stephens, Petreas, and Hayward (1995). U.S. EPA OSW recommends the following soil ingestion rate for chicken:

Recommended Value for: Quantity of Soil Eaten by the Animal (Chicken) Each Day (Qs)
0.022 kg DW/day

Uncertainties associated with this variable include the lack of current empirical data to support soil ingestion rates for chicken, and the assumption of uniform contamination of soil ingested by chicken.

5.6.1.5 Average Soil Concentration Over Exposure Duration (Cs)

The calculation of Cs for chicken is the same as for beef cattle (Section 5.4.4.5).

5.6.1.6 Soil Bioavailability Factor (Bs)

The calculation of Bs for chicken is the same as for beef cattle (Section 5.4.4.6)

5.7   CALCULATION OF COPC CONCENTRATIONS IN DRINKING WATER AND FISH

COPC concentrations in surface water are calculated for all water bodies selected for evaluation in the risk assessment; specifically, evaluation of the drinking water and/or fish ingestion exposure pathways. Mechanisms considered for determination of COPC loading of the water column are:

(1)   Direct deposition,

(2)   Runoff from impervious surfaces within the watershed,

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(3)   Runoff from pervious surfaces within the watershed,

(4)   Soil erosion over the total watershed,

(5)   Direct diffusion of vapor phase COPCs into the surface water, and

(6)   Internal transformation of compounds chemically or biologically.

Other potential mechanisms may require consideration on a case-by-case basis (e.g., tidal influences), however, contributions from other potential mechanisms are assumed to be negligible in comparison with those being evaluated.

The USLE and a sediment delivery ratio are used to estimate the rate of soil erosion from the watershed. Surface water concentration algorithms include a sediment mass balance, in which the amount of sediment assumed to be buried and lost from the water body is equal to the difference between the amount of soil introduced to the water body by erosion and the amount of suspended solids lost in downstream flow. As a result, the assumptions are made that sediments do not accumulate in the water body over time, and an equilibrium is maintained between the surficial layer of sediments and the water column. The total water column COPC concentration is the sum of the COPC concentration dissolved in water and the COPC concentration associated with suspended solids. Partitioning between water and sediment varies with the COPC. The total concentration of each COPC is partitioned between the sediment and the water column. The equations used to estimate surface water concentrations are presented in Appendix B-4. To evaluate the COPC loading to a water body from its associated watershed, the COPC concentration in watershed soils should be calculated. As described in Section 5.2, the equation for COPC concentration in soil includes a loss term that considers the loss of contaminants from the soil after deposition. These loss mechanisms all lower the soil concentration associated with a specific deposition rate.

Appendix B, Tables B-4-1 through B-4-28, provides equations for calculating COPC concentrations in watershed soils, and COPC concentrations in the water body.

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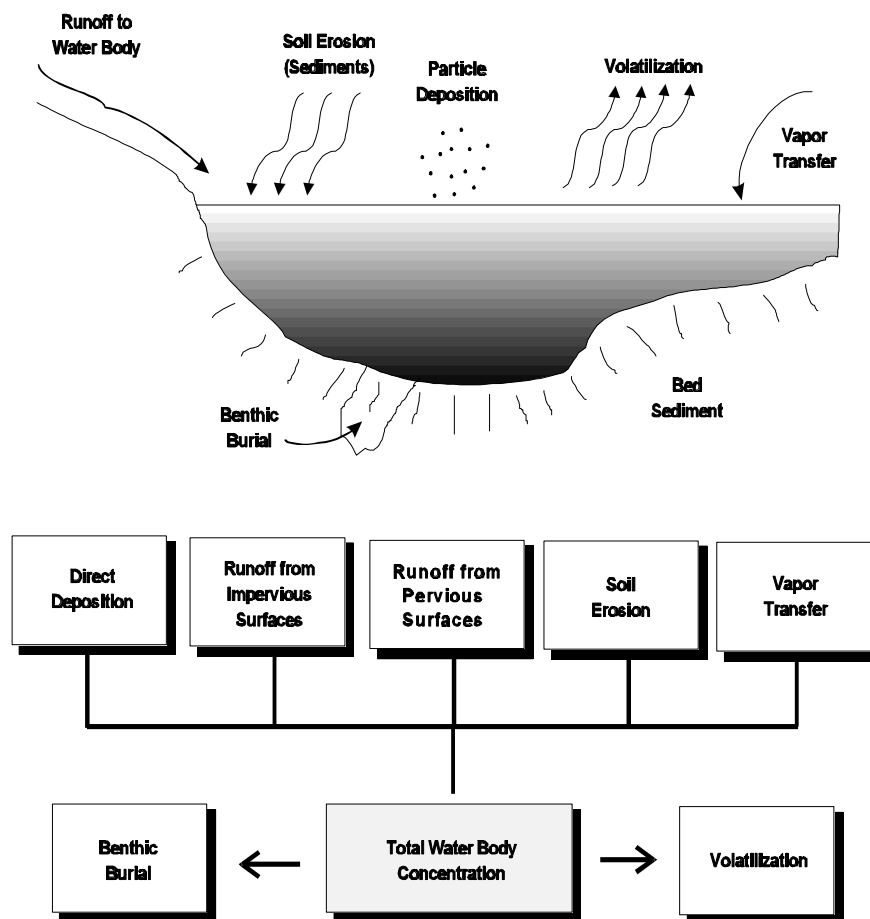
Figure 5-7 - COPC Loading to the Water Body

5.7.1   Total COPC Load to the Water Body (L_T)

Consistent with U.S. EPA (1994r) and NC DEHNR (1997), U.S. EPA OSW recommends the use of Equation 5-28 to calculate the total COPC load to a water body (L_T). This equation is described in detail in Appendix B, Table B-4-7.

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Recommended Equation for Calculating:
Total COPC Load to the Water Body (L_T)

$$L_T = L_{DEP} + L_{dif} + L_{RI} + L_R + L_E + L_I$$ Equation 5-28

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where

L_T	=	Total COPC load to the water body (including deposition, runoff, and erosion) (g/yr)
L_{DEP}	=	Total (wet and dry) particle phase and wet vapor phase COPC direct deposition load to water body (g/yr)
L_{dif}	=	Vapor phase COPC diffusion (dry deposition) load to water body (g/yr)
L_{RI}	=	Runoff load from impervious surfaces (g/yr)
L_R	=	Runoff load from pervious surfaces (g/yr)
L_E	=	Soil erosion load (g/yr)
L_I	=	Internal transfer (g/yr)

Due to the limited data and uncertainty associated with the chemical or biological internal transfer, L_I, of compounds into daughter products, U.S. EPA OSW recommends a default value for this variable of zero. However, if a permitting authority determines that site-specific conditions indicate calculation of internal transfer should be considered, U.S. EPA OSW recommends following the methodologies described in U.S. EPA NCEA document, *Methodology for Assessing Health Risks Associated with Multiple Exposure Pathways to Combustor Emissions* (In Press). Calculation of each of the remaining variables (L_{DEP}, L_{dif}, L_{RI}, L_R, and L_E) is discussed in the following subsections.

5.7.1.1 Total (Wet and Dry) Particle Phase and Wet Vapor Phase COPC Direct Deposition Load to Water Body (L_{DEP})

Consistent with U.S. EPA (1994r) and NC DEHNR (1997), U.S. EPA OSW recommends Equation 5-29 to calculate the load to the water body from the direct deposition of wet and dry particles and wet vapors onto the surface of the water body (L_{DEP}). The equation is described in detail in Appendix B, Table B-4-8.

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Recommended Equation for Calculating:

Total Particle Phase and Wet Vapor Phase Direct Deposition Load to Water Body (L_{DEP})

$$L_{DEP} = Q \cdot [\ F_v \cdot Dywwv + (1 - F_v)\cdot Dytwp\ ] \cdot A_W$$ Equation 5-29

---

where

L_{DEP}	=	Total (wet and dry) particle phase and wet vapor phase COPC direct deposition load to water body (g/yr)
Q	=	COPC emission rate (g/s)
F_v	=	Fraction of COPC air concentration in vapor phase (unitless)
$Dywwv$	=	Unitized yearly (water body and watershed) average wet deposition from vapor phase (s/m^2-yr)
$Dytwp$	=	Unitized yearly (water body and watershed) average total (wet and dry) deposition from vapor phase (s/m^2-yr)
A_W	=	Water body surface area (m^2)

Chapter 3 describes the determination of the modeled air parameters, $Dywwv$ and $Dywwv$. The determination of water body surface area, A_w, is described in Chapter 4 and Appendix B. Appendix A-3 describes determination of the compound-specific parameters, F_v.

5.7.1.2 Vapor Phase COPC Diffusion (Dry Deposition) Load to Water Body (L_{dif})

Consistent with U.S. EPA (1994r) and NC DEHNR (1997), U.S. EPA OSW recommends using Equation 5-30 to calculate the dry vapor phase COPC diffusion load to the water body (L_{dif}). The equation is described in detail in Appendix B, Table B-4-12.

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Recommended Equation for Calculating:
Vapor Phase COPC Diffusion (Dry Deposition) Load to Water Body (L_{Dif})

$$L_{dif} = \frac{K_v \cdot Q \cdot F_v \cdot Cywv \cdot A_W \cdot 1 \times 10^{-6}}{\dfrac{H}{R \cdot T_{wk}}}$$ Equation 5-30

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where

L_{dif}	=	Vapor phase COPC diffusion (dry deposition) load to water body (g/yr)
K_v	=	Overall COPC transfer rate coefficient (m/yr)
Q	=	COPC emission rate (g/s)
F_v	=	Fraction of COPC air concentration in vapor phase (unitless)
$Cywv$	=	Unitized yearly (water body and watershed) average air concentration from vapor phase (μg-s/g-m^3)
A_W	=	Water body surface area (m^2)
10^{-6}	=	Units conversion factor (g/μg)
H	=	Henry's Law constant (atm-m^3/mol)
R	=	Universal gas constant (atm-m^3/mol-K)
T_{wk}	=	Water body temperature (K)

The overall COPC transfer rate coefficient (K_v) is calculated by using Equation 5-40. The equation is also presented in Appendix B, Table B-4-19. Consistent with U.S. EPA (1994r) and U.S. EPA (1993h), U.S. EPA OSW recommends a water body temperature (T_{wk}) of 298 K (or 25°C). Chapter 3 describes the determination of the modeled air parameter, $Cywv$. The determination of water body surface area, A_w, is described in Chapter 4 and Appendix B. Appendix A-3 describes determination of compound-specific parameters, F_v, H, and R.

5.7.1.3 Runoff Load from Impervious Surfaces (L_{RI})

In some watershed soils, a fraction of the wet and dry deposition in the watershed will be to impervious surfaces. Dry deposition may accumulate and be washed off during rain events. Consistent with U.S. EPA (1994r) and NC DEHNR (1997), U.S. EPA OSW recommends the use of Equation 5-31 to calculate impervious runoff load to a water body (L_{RI}). The equation is also presented in Appendix B, Table B-4-9.

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Recommended Equation for Calculating:
Runoff Load from Impervious Surfaces (L_{RI})

$$L_{RI} = Q \cdot [\ F_v \cdot Dywwv + (1.0 - F_v) \cdot Dytwp\ ] \cdot A_I \qquad \text{Equation 5-31}$$

where

L_{RI}	$=$	Runoff load from impervious surfaces (g/yr)
Q	$=$	COPC emission rate (g/s)
F_v	$=$	Fraction of COPC air concentration in vapor phase (unitless)
$Dywwv$	$=$	Unitized yearly (water body and watershed) average wet deposition from vapor phase (s/m^2-yr)
$Dytwp$	$=$	Unitized yearly (water body and watershed) average total (wet and dry) deposition from vapor phase (s/m^2-yr)
A_I	$=$	Impervious watershed area receiving COPC deposition (m^2)

Impervious watershed area receiving COPC deposition (A_I) is the portion of the total effective watershed area that is impervious to rainfall (such as roofs, driveways, streets, and parking lots) and drains to the water body.

5.7.1.4 Runoff Load from Pervious Surfaces (L_R)

Consistent with U.S. EPA (1994r) and NC DEHNR (1997), U.S. EPA OSW recommends the use of Equation 5-32 to calculate the runoff dissolved COPC load to the water body from pervious soil surfaces in the watershed (L_R). The equation is also presented in Appendix B, Table B-4-10.

Recommended Equation for Calculating:
Runoff Load from Pervious Surfaces (L_R)

$$L_R = RO \cdot (A_L - A_I) \cdot \frac{Cs \cdot BD}{\theta_{sw} + Kd_s \cdot BD} \cdot 0.01 \qquad \text{Equation 5-32}$$

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where

L_R	=	Runoff load from pervious surfaces (g/yr)
RO	=	Average annual surface runoff from pervious areas (cm/yr)
A_L	=	Total watershed area receiving COPC deposition (m^2)
A_I	=	Impervious watershed area receiving COPC deposition (m^2)
Cs	=	Average soil concentration over exposure duration (in watershed soils) (mg COPC/kg soil)
BD	=	Soil bulk density (g soil/cm^3 soil)
θ_{sw}	=	Soil volumetric water content (mL water/cm^3 soil)
Kd_s	=	Soil-water partition coefficient (cm^3 water/g soil)
0.01	=	Units conversion factor (kg-cm^2/mg-m^2)

Appendix B describes the determination of site-specific parameters, RO, A_L, A_I, BD, and θ_{sw}. The calculation of the COPC concentration in watershed soils (Cs) are discussed in Section 5.2.1 and Appendix B, Table B-4-1. Soil bulk density (BD) is described in Section 5.2.5.2. Soil water content (θ_{sw}) is described in Section 5.2.5.4.

5.7.1.5 Soil Erosion Load (L_E)

Consistent with U.S. EPA (1994r) and NC DEHNR (1997), U.S. EPA OSW recommends the use of Equation 5-33 to calculate soil erosion load (L_E). The equation is also presented in Appendix B, Table B-4-11.

Recommended Equation for Calculating:
Soil Erosion Load (L_E)

$$L_E = X_e \cdot (A_L - A_I) \cdot SD \cdot ER \cdot \frac{Cs \cdot Kd_s \cdot BD}{\theta_{sw} + Kd_s \cdot BD} \cdot 0.001$$ Equation 5-33

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where

L_E	=	Soil erosion load (g/yr)
X_e	=	Unit soil loss (kg/m^2-yr)
A_L	=	Total watershed area (evaluated) receiving COPC deposition (m^2)
A_I	=	Impervious watershed area receiving COPC deposition (m^2)
SD	=	Sediment delivery ratio (watershed) (unitless)

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ER	=	Soil enrichment ratio (unitless)
Cs	=	Average soil concentration over exposure duration (in watershed soils) (mg COPC/kg soil)
BD	=	Soil bulk density (g soil/cm^3 soil)
θ_{sw}	=	Soil volumetric water content (mL water/cm^3 soil)
Kd_s	=	Soil-water partition coefficient (mL water/g soil)
0.001	=	Units conversion factor (k-cm^2/mg-m^2)

Unit soil loss (X_e) is described in Section 5.7.2. Watershed sediment delivery ratio (*SD*) is calculated as described in Section 5.7.3 and in Appendix B, Table B-4-14. COPC concentration in soils (*Cs*) is described in Section 5.2.1, and Appendix B, Table B-4-1. Soil bulk density (*BD*) is described in Section 5.2.5.2. Soil water content (θ_{sw}) is described in Section 5.2.5.4.

5.7.2   Universal Soil Loss Equation - USLE

U.S. EPA OSW recommends that the universal soil loss equation (USLE), Equation 5-33A, be used to calculate the unit soil loss *(X$_e$)* specific to each watershed. This equation is further described in Appendix B, Table B-4-13. Appendix B also describes determination of the site- and watershed-specific values for each of the variables associated with Equation 5-33A. The use of Equation 5-33A is consistent with U.S. EPA (1994g) and U.S. EPA (1994r).

Recommended Equation for Calculating:
Unit Soil Loss (X_e)

$$X_e = RF \cdot K \cdot LS \cdot C \cdot PF \cdot \frac{907.18}{4047}$$

Equation 5-33A

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where

X_e	=	Unit soil loss (kg/m^2-yr)
RF	=	USLE rainfall (or erosivity) factor (yr^{-1})
K	=	USLE erodibility factor (ton/acre)
LS	=	USLE length-slope factor (unitless)
C	=	USLE cover management factor (unitless)
PF	=	USLE supporting practice factor (unitless)
907.18	=	Units conversion factor (kg/ton)

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4047   =   Units conversion factor (m^2/acre)

The USLE *RF* variable, which represents the influence of precipitation on erosion, is derived from data

on the frequency and intensity of storms. This value is typically derived on a storm-by-storm basis, but

average annual values have been compiled (U.S. Department of Agriculture 1982). Information on

determining site-specific values for variables used in calculating X_e is provided in U.S. Department of

Agriculture (U.S. Department of Agriculture 1997) and U.S. EPA guidance (U.S. EPA 1985b).

Refer to Appendix B, Table B-4-13 for additional discussion of the USLE.

5.7.3   Sediment Delivery Ratio (*SD*)

U.S. EPA OSW recommends the use of Equation 5-34 to calculate sediment delivery ratio (*SD*). The use

of this equation is further described in Appendix B, Table B-4-14.

Recommended Equation for Calculating:
Sediment Delivery Ratio *(SD)*

$$SD \ = \ a \cdot (A_L \ )^{-b}$$ Equation 5-34

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where

SD	=	Sediment delivery ratio (watershed) (unitless)
a	=	Empirical intercept coefficient (unitless)
b	=	Empirical slope coefficient (unitless)
A_L	=	Total watershed area (evaluated) receiving COPC deposition (m^2)

The sediment delivery ratio (*SD*) for a large land area, a watershed or part of a watershed, can be

calculated, on the basis of the area of the watershed, by using an approach proposed by Vanoni (1975).

Accordingly, U.S. EPA (1993h) recommended the use of Equation 5-34 to calculate the sediment

delivery ratio.

According to Vanoni (1975), sediment delivery ratios vary approximately with the -0.125 power of the

drainage area. Therefore, the empirical slope coefficient is assumed to be equal to 0.125. An inspection

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of the data presented by Vanoni (1975) indicates that the empirical intercept coefficient varies with the

size of the watershed, as illustrated in Appendix B, Table B-4-14.

A_L is the total watershed surface area evaluated that is affected by deposition and drains to the body of

water (see Chapter 4). In assigning values to the watershed surface area affected by deposition, the

following may be a consideration:

> (1)   the distance from the emission source,

> (2)   the location of the area affected by deposition fallout with respect to the point at which
>   drinking water is extracted or fishing occurs

> (3)   the watershed hydrology.

5.7.4   Total Water Body COPC Concentration (C_{wtot})

U.S. EPA OSW recommends the use of Equation 5-35 to calculate total water body COPC concentration

(C_{wtot}). The total water body concentration includes both the water column and the bed sediment. The

equation is also presented in Appendix B, Table B-4-15.

Recommended Equation for Calculating:
Total Water Body COPC Concentration (C_{wtot})

$$C_{wtot} = \frac{L_T}{Vf_x \cdot f_{wc} + k_{wt} \cdot A_W \cdot (d_{wc} + d_{bs})}$$

Equation 5-35

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where

C_{wtot}	=	Total water body COPC concentration (including water column and bed sediment) (g COPC/m^3 water body)
L_T	=	Total COPC load to the water body (including deposition, runoff, and erosion) (g/yr)
Vf_x	=	Average volumetric flow rate through water body (m^3/yr)
f_{wc}	=	Fraction of total water body COPC concentration in the water column (unitless)
k_{wt}	=	Overall total water body COPC dissipation rate constant (yr^{-1})

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A_W	=	Water body surface area (m^2)
d_{wc}	=	Depth of water column (m)
d_{bs}	=	Depth of upper benthic sediment layer (m)

The total COPC load to the water body (L_T)—including deposition, runoff, and erosion—is described in Section 5.7.1 and Appendix B, Table B-4-7. The depth of the upper benthic layer (d_{bs}), which represents the portion of the bed that is in equilibrium with the water column, cannot be precisely specified; however, U.S. EPA (1993h) recommended values ranging from 0.01 to 0.05. Consistent with U.S. EPA (1994r), U.S. EPA OSW recommends a default value of 0.03, which represents the midpoint of the specified range. Issues related to the remaining parameters are summarized in the following subsections.

5.7.4.1 Fraction of Total Water Body COPC Concentration in the Water Column (f_{wc}) and Benthic Sediment (f_{bs})

U.S. EPA OSW recommends using Equation 5-36A to calculate fraction of total water body COPC concentration in the water column (f_{wc}), and Equation 5-36B to calculate total water body contaminant concentration in benthic sediment (f_{bs}). The equations are also presented in Appendix B, Table B-4-16.

Recommended Equation for Calculating:
Fraction of Total Water Body COPC Concentration in
the Water Column (f_{wc}) and Benthic Sediment (f_{bs})

$$f_{wc} = \frac{(1 + Kd_{sw} \cdot TSS \cdot 1 \times 10^{-6}) \cdot d_{wc}/d_z}{(1 + Kd_{sw} \cdot TSS \cdot 1 \times 10^{-6}) \cdot d_{wc}/d_z + (\theta_{bs} + Kd_{bs} \cdot C_{BS}) \cdot d_{bs}/d_z}$$

Equation 5-36A

$$f_{bs} = 1 - f_{wc}$$

Equation 5-36B

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where

f_{wc}	=	Fraction of total water body COPC concentration in the water column (unitless)
f_{bs}	=	Fraction of total water body COPC concentration in benthic sediment (unitless)

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Kd_{sw}	=	Suspended sediments/surface water partition coefficient (L water/kg suspended sediment)
TSS	=	Total suspended solids concentration (mg/L)
1×10^{-6}	=	Units conversion factor (kg/mg)
d_z	=	Total water body depth (m)
θ_{bs}	=	Bed sediment porosity ($L_{water}/L_{sediment}$)
Kd_{bs}	=	Bed sediment/sediment pore water partition coefficient (L water/kg bottom sediment)
C_{BS}	=	Bed sediment concentration (g/cm^3 [equivalent to kg/L])
d_{wc}	=	Depth of water column (m)
d_{bs}	=	Depth of upper benthic sediment layer (m)

U.S. EPA (1993h) and NC DEHNR (1997) recommended the use of Equations 5-36A and 5-36B to calculate the fraction of total water body concentration occurring in the water column (f_{wc}) and the bed sediments (f_{bs}). The partition coefficient Kd_{sw} describes the partitioning of a contaminant between sorbing material, such as soil, surface water, suspended solids, and bed sediments (see Appendix A-3). NC DEHNR (1997) also recommended adding the depth of the water column to the depth of the upper benthic layer ($d_{wc} + d_{bs}$) to calculate the total water body depth (d_z).

NC DEHNR (1997) recommended a default total suspended solids (TSS) concentration of 10 mg/L, which was adapted from U.S. EPA (1993g). However, due to variability in water body specific values for this variable, U.S. EPA OSW recommends the use of water body-specific measured TSS values representative of long-term average annual values for the water body of concern. Average annual values for TSS are generally expected to be in the range of 2 to 300 mg/L; with additional information on anticipated TSS values available in the U.S. EPA NCEA document, *Methodology for Assessing Health Risks Associated with Multiple Exposure Pathways to Combustor Emissions* (In Press).

If measured data is not available, or of unacceptable quality, a calculated TSS value can be obtained for non-flowing water bodies using Equation 5-36C.

$$TSS = \frac{X_e \cdot (A_L - A_I) \cdot SD \cdot 1x10^3}{Vf_x + D_{ss} \cdot A_W}$$ Equation 5-36C

where

TSS	=	Total suspended solids concentration (mg/L)
X_e	=	Unit soil loss (kg/m^2-yr)

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A_L	=	Total watershed area (evaluated) receiving COPC deposition (m^2)
A_I	=	Impervious watershed area receiving COPC deposition (m^2)
SD	=	Sediment delivery ratio (watershed) (unitless)
Vf_x	=	Average volumetric flow rate through water body (value should be 0 for quiescent lakes or ponds) (m^3/yr)
D_{ss}	=	Suspended solids deposition rate (a default value of 1,825 for quiescent lakes or ponds) (m/yr)
A_W	=	Water body surface area (m^2)

The default value of 1,825 m/yr provided for D_{ss} is characteristic of Stoke's settling velocity for an intermediate (fine to medium) silt.

Also, to evaluate the appropriateness of watershed-specific values used in calculating the unit soil loss (X_e), as described in Section 5.7.2 and Appendix B, the water-body specific measured *TSS* value should be compared to the calculated *TSS* value obtained using Equation 5-36C. If the measured and calculated *TSS* values differ significantly, parameter values used in calculating X_e should be re-evaluated. This re-evaluation of *TSS* and X_e should also be conducted if the calculated *TSS* value is outside of the normal range expected for average annual measured values, as discussed above.

Bed sediment porosity (θ_{bs}) can be calculated from the bed sediment concentration by using the following equation (U.S. EPA 1993h):

$$\theta_{bs} \; = \; 1 \; - \; \frac{C_{BS}}{\rho_s} \qquad\qquad\qquad \text{Equation 5-37}$$

where

θ_{bs}	=	Bed sediment porosity (L$_{water}$/L$_{sediment}$)
ρ_s	=	Bed sediment density (kg/L)
C_{BS}	=	Bed sediment concentration (kg/L)

U.S. EPA OSW recommends the following default value for bed sediment porosity (θ_{bs}), which was adapted from U.S. EPA (1993h) and NC DEHNR (1997):

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Recommended Value for:
Bed Sediment Porosity (θ_{bs})

$$\theta_{bs} = 0.6 \ \ L_{water}/L_{sediment}$$

(assuming $\rho_s = 2.65$ kg/L [bed sediment density] and $C_{BS} = 1$ kg/L [bed sediment concentration])

Concentrations for the bed sediment (C_{BS}) and depth of upper benthic sediment layer (d_{bs}) range from 0.5 to 1.5 meters and 0.01 to 0.05 meters, respectively. However, in accordance with U.S. EPA (1993h), U.S. EPA (1994r) and NC DEHNR (1997), 0.1 kg/L is a reasonable concentration for most applications of the bed sediment (C_{BS}), and 0.03 meter is the default depth of the upper benthic layer (d_{bs}). The default depth of 0.03 meters is based on the midpoint of the range presented above.

5.7.4.2 Overall Total Water Body COPC Dissipation Rate Constant (k_{wt})

Consistent with U.S. EPA (1994r) and NC DEHNR (1997), U.S. EPA OSW recommends the use of Equation 5-38 to calculate the overall dissipation rate of COPCs in surface water, resulting from volatilization and benthic burial. The equation is also presented in Appendix B, Table B-4-17.

Recommended Equation for Calculating:
Overall Total Water Body COPC Dissipation Rate Constant (k_{wt})

$$k_{wt} \ = \ f_{wc} \ \cdot \ k_v \ + \ f_{bs} \ \cdot \ k_b \qquad\qquad \text{Equation 5-38}$$

---

where

k_{wt}	=	Overall total water body dissipation rate constant (yr^{-1})
f_{wc}	=	Fraction of total water body COPC concentration in the water column (unitless)
k_v	=	Water column volatilization rate constant (yr^{-1})
f_{bs}	=	Fraction of total water body COPC concentration in benthic sediment (unitless)
k_b	=	Benthic burial rate constant (yr^{-1})

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The variables f_{wc} and f_{bs} are discussed in Section 5.7.4.1, Equations 5-36A and 5-36B, and calculated by using the equations presented in Appendix B, Table B-4-16.

5.7.4.3 Water Column Volatilization Rate Constant (k_v)

Consistent with U.S. EPA (1994r) and NC DEHNR (1997), U.S. EPA OSW recommends using Equation 5-39 to calculate water column volatilization rate constant. The equation is also presented in Appendix B, Table B-4-18.

Recommended Equation for Calculating:
Water Column Volatilization Rate Constant (k_v)

$$k_v = \frac{K_v}{d_z \cdot (1 + Kd_{sw} \cdot TSS \cdot 1 \times 10^{-6})}$$

Equation 5-39

---

where

k_v	=	Water column volatilization rate constant (yr^{-1})
K_v	=	Overall COPC transfer rate coefficient (m/yr)
d_z	=	Total water body depth (m)
Kd_{sw}	=	Suspended sediments/surface water partition coefficient (L water/kg suspended sediments)
TSS	=	Total suspended solids concentration (mg/L)
1×10^{-6}	=	Units conversion factor (kg/mg)

Total water body depth (d_z), suspended sediment and surface water partition coefficient (Kd_{sw}), and total suspended solids concentration (TSS), are described in Section 5.7.4.1. Kd_{sw} is also discussed in Appendix A-3. The overall transfer rate coefficient (K_v) is described in Section 5.7.4.4.

5.7.4.4 Overall COPC Transfer Rate Coefficient (K_v)

Volatile organic chemicals can move between the water column and the overlying air. The overall transfer rate K_v, or conductivity, is determined by a two-layer resistance model that assumes that two "stagnant films" are bounded on either side by well-mixed compartments. Concentration differences

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serve as the driving force for the water layer diffusion. Pressure differences drive the diffusion for the air

layer. From balance considerations, the same mass must pass through both films; the two resistances

thereby combine in series, so that the conductivity is the reciprocal of the total resistance.

Consistent with U.S. EPA (1993h), U.S. EPA (1993g), and NC DEHNR (1997), U.S. EPA OSW

recommends the use of Equation 5-40 to calculate the overall transfer rate coefficient (K_v). The equation

is also presented in Appendix B, Table B-4-19.

Recommended Equation for Calculating:
Overall COPC Transfer Rate Coefficient (K_v)

$$K_v = \left(K_L^{-1} + \left(K_G \cdot \frac{H}{R \cdot T_{wk}} \right)^{-1} \right)^{-1} \cdot \theta^{T_{wk} - 293}$$

Equation 5-40

---

where

K_v	=	Overall COPC transfer rate coefficient (m/yr)
K_L	=	Liquid phase transfer coefficient (m/yr)
K_G	=	Gas phase transfer coefficient (m/yr)
H	=	Henry's Law constant (atm-m^3/mol)
R	=	Universal gas constant (atm-m^3/mol-K)
T_{wk}	=	Water body temperature (K)
θ	=	Temperature correction factor (unitless)

The value of the conductivity K_v depends on the intensity of turbulence in the water body and the

overlying atmosphere. As Henry's Law constant increases, the conductivity tends to be increasingly

influenced by the intensity of turbulence in water. Conversely, as Henry's Law constant decreases, the

value of the conductivity tends to be increasingly influenced by the intensity of atmospheric turbulence.

The liquid and gas phase transfer coefficients, K_L and K_G, respectively, vary with the type of water body.

The liquid phase transfer coefficient (K_L) is calculated by using Equations 5-41A and 5-41B (described in

Section 5.7.4.5). The gas phase transfer coefficient (K_G) is calculated by using Equations 5-42A and

5-42B (described in Section 5.7.4.6).

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Henry's Law constants generally increase with increasing vapor pressure of a COPC and generally decrease with increasing solubility of a COPC. Henry's Law constants are compound-specific and are presented in Appendix A-3. The universal ideal gas constant, R, is 8.205×10^{-5} atm-m^3/mol-K, at 20°C. The temperature correction factor (θ), which is equal to 1.026, is used to adjust for the actual water temperature. Volatilization is assumed to occur much less readily in lakes and reservoirs than in moving water bodies.

5.7.4.5 Liquid Phase Transfer Coefficient (K_L)

U.S. EPA OSW recommends using Equations 5-41A and 5-41B to calculate liquid phase transfer coefficient. (K_L). The use of these equations is further described in Appendix B, Table B-4-20.

Recommended Equation for Calculating:
Liquid Phase Transfer Coefficient (K_L)

For flowing streams or rivers:

$$K_L = \sqrt{\frac{(1 \times 10^{-4}) \cdot D_w \cdot u}{d_z}} \cdot 3.1536 \times 10^7 \qquad \text{Equation 5-41A}$$

For quiescent lakes or ponds:

$$K_L = (C_d^{0.5} \cdot W) \cdot (\frac{\rho_a}{\rho_w})^{0.5} \cdot \frac{k^{0.33}}{\lambda_z} \cdot (\frac{\mu_w}{\rho_w \cdot D_w})^{-0.67} \cdot 3.1536 \times 10^7 \qquad \text{Equation 5-41B}$$

---

where

K_L	=	Liquid phase transfer coefficient (m/yr)
D_w	=	Diffusivity of COPC in water (cm^2/s)
u	=	Current velocity (m/s)
1×10^{-4}	=	Units conversion factor (m^2/cm^2)
d_z	=	Total water body depth (m)
C_d	=	Drag coefficient (unitless)
W	=	Average annual wind speed (m/s)
ρ_a	=	Density of air (g/cm^3)
ρ_w	=	Density of water (g/cm^3)
k	=	von Karman's constant (unitless)

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λ_z = Dimensionless viscous sublayer thickness (unitless)
μ_w = Viscosity of water corresponding to water temperature (g/cm-s)
3.1536 x 10^7 = Units conversion factor (s/yr)

For a flowing stream or river, the transfer coefficients are controlled by flow-induced turbulence. For these systems, the liquid phase transfer coefficient is calculated by using Equation 5-41A, which is the O'Connor and Dobbins (1958) formula, as presented in U.S. EPA (1993h).

For a stagnant system (quiescent lake or pond), the transfer coefficient is controlled by wind-induced turbulence. For quiescent lakes or ponds, the liquid phase transfer coefficient can be calculated by using Equation 5-41B (O'Connor 1983; U.S. EPA 1993h).

The total water body depth (d_z) for liquid phase transfer coefficients is discussed in Section 5.7.4.1.

Consistent with U.S. EPA (1994r) and NC DEHNR (1997), U.S. EPA OSW recommends the use of the following default values. These values are further described in Appendix A-3:

(1) a diffusivity of chemical in water ranging (D_w) from 1.0×10^{-5} to 8.5×10^{-2} cm²/s,

(2) a dimensionless viscous sublayer thickness (λ_z) of 4,

(3) a von Karman's constant (k) of 0.4,

(4) a drag coefficient (C_d) of 0.0011 which was adapted from U.S. EPA (1993h),

(5) a density of air (ρ_a) of 0.0012 g/cm³ at standard conditions (temperature = 20°C or 293 K, pressure = 1 atm or 760 millimeters of mercury) (Weast 1986),

(6) a density of water (ρ_w) of 1 g/cm³ (Weast 1986),

(7) a viscosity of water (μ_w) of a 0.0169 g/cm-s corresponding to water temperature (Weast 1986).

5.7.4.6 Gas Phase Transfer Coefficient (K_G)

U.S. EPA OSW recommends using Equations 5-42A and 5-42B to calculate gas phase transfer coefficient (K_G). The equation is also discussed in Appendix B, Table B-4-21.

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Recommended Equation for Calculating:
Gas Phase Transfer Coefficient (K_G)

For flowing streams or rivers:

$$K_G = 36500 \ \text{m/yr}$$ Equation 5-42A

For quiescent lakes or ponds:

$$K_G = (C_d^{0.5} \cdot W) \cdot \frac{k^{0.33}}{\lambda_z} \cdot (\frac{\mu_a}{\rho_a \cdot D_a})^{-0.67} \cdot 3.1536 \times 10^7$$ Equation 5-42B

---

where

K_G	=	Gas phase transfer coefficient (m/yr)
C_d	=	Drag coefficient (unitless)
W	=	Average annual wind speed (m/s)
k	=	von Karman's constant (unitless)
λ_z	=	Dimensionless viscous sublayer thickness (unitless)
μ_a	=	Viscosity of air corresponding to air temperature (g/cm-s)
ρ_a	=	Density of air corresponding to water temperature (g/cm^3)
D_a	=	Diffusivity of COPC in air (cm^2/s)
3.1536×10^7	=	Units conversion factor (s/yr)

U.S. EPA (1993h) indicated that the rate of transfer of a COPC from the gas phase for a flowing stream or river is assumed to be constant, in accordance with O'Connor and Dobbins (1958) (Equation 5-42A).

For a stagnant system (quiescent lake or pond), the transfer coefficients are controlled by wind-induced turbulence. For quiescent lakes or ponds, U.S. EPA OSW recommends that the gas phase transfer coefficient be computed by using the equation presented in O'Connor (1983) (Equation 5-42B).

Consistent with U.S. EPA (1994r) and NC DEHNR (1997), U.S. EPA OSW recommends 1.81 x 10^{-4} g/cm-s for the viscosity of air corresponding to air temperature.

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5.7.4.7 Benthic Burial Rate Constant (k_b)

U.S. EPA OSW recommends using Equation 5-43 to calculate benthic burial rate (k_b). The equation is also discussed in Appendix B, Table B-4-22.

Recommended Equation for Calculating:
Benthic Burial Rate Constant (k_b)

$$k_b = \left(\frac{X_e \cdot A_L \cdot SD \cdot 1 \times 10^3 - Vf_x \cdot TSS}{A_W \cdot TSS} \right) \cdot \left(\frac{TSS \cdot 1 \times 10^{-6}}{C_{BS} \cdot d_{bs}} \right) \qquad \text{Equation 5-43}$$

---

where

k_b	=	Benthic burial rate constant (yr^{-1})
X_e	=	Unit soil loss (kg/m²-yr)
A_L	=	Total watershed area (evaluated) receiving deposition (m²)
SD	=	Sediment delivery ratio (watershed) (unitless)
Vf_x	=	Average volumetric flow rate through water body (m³/yr)
TSS	=	Total suspended solids concentration (mg/L)
A_W	=	Water body surface area (m²)
C_{BS}	=	Bed sediment concentration (g/cm³)
d_{bs}	=	Depth of upper benthic sediment layer (m)
1×10^{-6}	=	Units conversion factor (kg/mg)
1×10^3	=	Units conversion factor (g/kg)

The benthic burial rate constant (k_b), which is calculated in Equation 5-43, can also be expressed in terms of the rate of burial (Wb):

$$Wb = k_b \cdot d_{bs} \qquad \text{Equation 5-44}$$

where

Wb	=	Rate of burial (m/yr)
k_b	=	Benthic burial rate constant (yr^{-1})
d_{bs}	=	Depth of upper benthic sediment layer (m)

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According to U.S. EPA (1994r) and NC DEHNR (1997), COPC loss from the water column resulting from burial in benthic sediment can be calculated by using Equation 5-43. U.S. EPA (1994r) and NC DEHNR (1997) recommended a benthic solids concentration (C_{BS}) ranging from 0.5 to 1.5 kg/L, which was adapted from U.S. EPA (1993g). U.S. EPA OSW recommends the following default value for bed sediment concentration (C_{BS}).

Recommended Default Value for:
Bed Sediment Concentration (C_{BS})
1.0 kg/L

Section 5.7.2 discusses the unit soil loss (X_e). Section 5.7.3 discusses sediment delivery ratio (SD) and watershed area evaluated receiving COPC deposition (A_L). Section 5.7.4 discusses the depth of the upper benthic sediment layer (d_{bs}). Average volumetric flow rate through the water body (Vf_x) and water body surface area (A_w) are discussed in Appendix B. A_w is also discussed in Appendix A-3. Section 5.7.4.1 discusses total suspended solids concentration (TSS).

The calculated value for k_b should range from 0 to 1.0; with low k_b values expected for water bodies characteristic of no or limited sedimentation (rivers and fast flowing streams), and k_b values closer to 1.0 expected for water bodies characteristic of higher sedimentation (lakes). This range of values is based on the relation between the benthic burial rate and rate of burial expressed in Equation 5-44; with the depth of upper benthic sediment layer held constant. For k_b values calculated as a negative (water bodies with high average annual volumetric flow rates in comparison to watershed area evaluated), a k_b value of 0 should be assigned for use in calculating the total water body COPC concentration (C_{wtot}) in Equation 5-35. If the calculated k_b value exceeds 1.0, re-evaluation of the parameter values used in calculating X_e should be conducted.

5.7.4.8 Total COPC Concentration in Water Column (C_{wctot})

U.S. EPA OSW recommends using Equation 5-45 to calculate total COPC concentration in water column (C_{wctot}). The equation is also discussed in Appendix B, Table B-4-23.

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Recommended Equation for Calculating:		
Total COPC Concentration in Water Column (C_{wctot})		

$$C_{wctot} = f_{wc} \cdot C_{wtot} \cdot \frac{d_{wc} + d_{bs}}{d_{wc}}$$ Equation 5-45

---

where

C_{wctot}	=	Total COPC concentration in water column (mg COPC/L water column)
f_{wc}	=	Fraction of total water body COPC concentration in the water column (unitless)
C_{wtot}	=	Total water body COPC concentration, including water column and bed sediment (mg COPC/L water body)
d_{wc}	=	Depth of water column (m)
d_{bs}	=	Depth of upper benthic sediment layer (m)

The use of Equation 5-45 to calculate total COPC concentration in water column is consistent with U.S. EPA (1994r) and NC DEHNR (1997).

Total water body COPC concentration—including water column and bed sediment (C_{wtot}) and fraction of total water body COPC concentration in the water column (f_{wc})—should be calculated by using Equation 5-35 (also see Appendix B, Table B-4-15) and Equation 5-36A (also see Appendix B, Table B-4-16), respectively. Depth of upper benthic sediment layer (d_{bs}) is discussed in Section 5.7.4.1.

5.7.4.9 Dissolved Phase Water Concentration (C_{dw})

U.S. EPA OSW recommends the use of Equation 5-46 to calculate the concentration of COPC dissolved in the water column (C_{dw}). The equation is discussed in detail in Appendix B, Table B-4-24.

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Recommended Equation for Calculating:
Dissolved Phase Water Concentration (C_{dw})

$$C_{dw} = \frac{C_{wctot}}{1 + Kd_{sw} \cdot TSS \cdot 1 \times 10^{-6}}$$

Equation 5-46

---

where

C_{dw}	=	Dissolved phase water concentration (mg COPC/L water)
C_{wctot}	=	Total COPC concentration in water column (mg COPC/L water column)
Kd_{sw}	=	Suspended sediments/surface water partition coefficient (L water/kg suspended sediment)
TSS	=	Total suspended solids concentration (mg/L)
1×10^{-6}	=	Units conversion factor (kg/mg)

The use of Equation 5-46 to calculate the concentration of COPC dissolved in the water column is consistent with U.S. EPA (1994r) and NC DEHNR (1997).

The total COPC concentration in water column (C_{wctot}) is calculated by using the Equation 5-45 (see also Appendix B, Table B-4-23). Section 5.7.4.1 discusses the surface water partition coefficient (Kd_{sw}) and total suspended solids concentration (TSS).

5.7.4.10   COPC Concentration Sorbed to Bed Sediment (C_{sb})

U.S. EPA OSW recommends the use of Equation 5-47 to calculate COPC concentration sorbed to bed sediment (C_{sb}). The equation is also presented in Appendix B, Table B-4-25.

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Recommended Equation for Calculating:
COPC Concentration Sorbed to Bed Sediment (C_{sb})

$$C_{sb} = f_{bs} \cdot C_{wtot} \cdot \left(\frac{Kd_{bs}}{\theta_{bs} + Kd_{bs} \cdot C_{BS}} \right) \cdot \left(\frac{d_{wc} + d_{bs}}{d_{bs}} \right)$$ Equation 5-47

where

C_{sb}	=	COPC concentration sorbed to bed sediment (mg COPC/kg sediment)
f_{bs}	=	Fraction of total water body COPC concentration in benthic sediment (unitless)
C_{wtot}	=	Total water body COPC concentration, including water column and bed sediment (mg COPC/L water body)
Kd_{bs}	=	Bed sediment/sediment pore water partition coefficient (L COPC/kg water body)
θ_{bs}	=	Bed sediment porosity ($L_{pore\ water}/L_{sediment}$)
C_{BS}	=	Bed sediment concentration (g/cm^3)
d_{wc}	=	Depth of water column (m)
d_{bs}	=	Depth of upper benthic sediment layer (m)

The use of Equation 5-47 to calculate the COPC concentration sorbed to bed sediment is consistent with U.S. EPA (1994r) and NC DEHNR (1997).

The total water body COPC concentration—including water column and bed sediment (C_{wtot}) and the fraction of total water body COPC concentration that occurs in the benthic sediment (f_{bs})—is calculated by using the equations in Appendix B, Tables B-4-15 and B-4-16, respectively. Bed sediment and sediment pore water partition coefficient (Kd_{bs}) is discussed in Appendix A-3. Bed sediment porosity (θ_{bs}) and bed sediment concentration (C_{BS}) are discussed in Section 5.7.4.1. Depth of water column (d_{wc}) and depth of upper benthic layer (d_{bs}) are discussed in Section 5.7.4.

5.7.5   Concentration of COPC in Fish (C_{fish})

The COPC concentration in fish is calculated using either a COPC-specific bioconcentration factor (*BCF*), a COPC-specific bioaccumulation factor (*BAF*), or a COPC-specific biota-sediment accumulation factor (*BSAF*). For compounds with a *log K_{ow}* less than 4.0, *BCF*s are used.

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Compounds with a $log\ K_{ow}$ greater than 4.0 (except for extremely hydrophobic compounds such as dioxins, furans, and PCBs), are assumed to have a high tendency to bioaccumulate, therefore, *BAF*s are used. While extremely hydrophobic COPCs like dioxins, furans, and PCBs are also assumed to have a high tendency to bioaccumulate, they are expected to be sorbed to the bed sediments more than associated with the water phase. Therefore, for dioxins, furans, and PCBs, *BSAF*s were used to calculate concentrations in fish. Appendix A-3, provides a detailed discussion on the sources of the COPC-specific *BCF*, *BAF*, and *BSAF* values, and the methodology used to derive them.
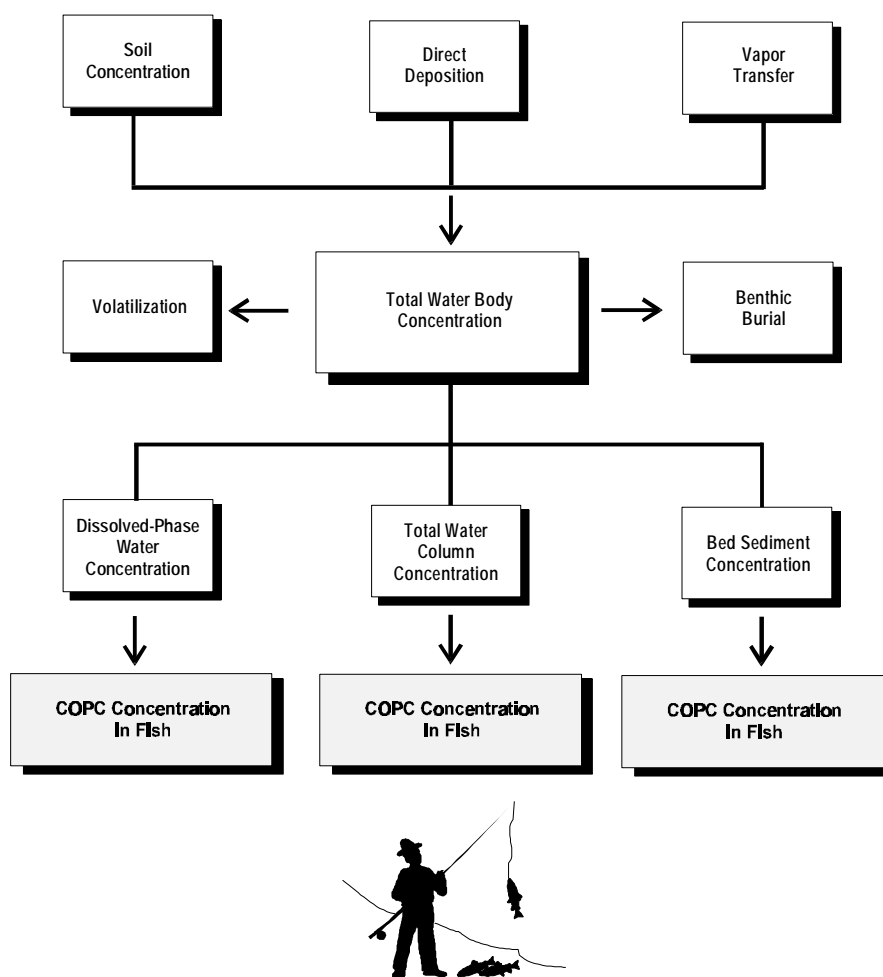

Figure 5-8 - COPC Concentration in Fish

BCF and *BAF* values are generally based on dissolved water concentrations. Therefore, when *BCF* or *BAF* values are used, the COPC concentration in fish is calculated using dissolved water concentrations. *BSAF* values are based on benthic sediment concentrations. Therefore, when *BSAF* values are used,

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COPC concentration in fish is calculated using benthic sediment concentrations. The equations used to calculate fish concentrations are described in the subsequent subsections.

5.7.5.1 Fish Concentration (C_{fish}) from Bioconcentration Factors Using Dissolved Phase Water Concentration

U.S. EPA OSW recommends the use of Equation 5-48 to calculate fish concentration from *BCF*s using dissolved phase water concentration. The use of this equation is further described in Appendix B, Table B-4-26.

Recommended Equation for Calculating:
Fish Concentration (C_{fish}) from Bioconcentration Factors (BCF_{fish})
Using Dissolved Phase Water Concentration

$$C_{fish} = C_{dw} \cdot BCF_{fish}$$

Equation 5-48

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where

C_{fish}	=	Concentration of COPC in fish (mg COPC/kg FW tissue)
C_{dw}	=	Dissolved phase water concentration (mg COPC/L)
BCF_{fish}	=	Bioconcentration factor for COPC in fish (L/kg)

The dissolved phase water concentration (C_{dw}) is calculated by using the Equation 5-46. COPC-specific BCF_{fish} values are presented in Appendix A-3.

The use of Equation 5-48 to calculate fish concentration is consistent with U.S. EPA (1994r) and NC DEHNR (1997).

5.7.5.2 Fish Concentration (C_{fish}) from Bioaccumulation Factors Using Dissolved Phase Water Concentration

U.S. EPA OSW recommends the use of Equation 5-49 to calculate fish concentration from *BAF*s using dissolved phase water concentration. The equation is also presented in Appendix B, Table B-4-27.

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Recommended Equation for Calculating:
Fish Concentration (C_{fish}) from Bioaccumulation Factors (BAF_{fish})
Using Dissolved Phase Water Concentration

$$C_{fish} = C_{dw} \cdot BAF_{fish}$$ Equation 5-49

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where

C_{fish}	=	Concentration of COPC in fish (mg COPC/kg FW tissue)
C_{dw}	=	Dissolved phase water concentration (mg COPC/L)
BAF_{fish}	=	Bioaccumulation factor for COPC in fish (L/kg FW tissue)

The dissolved phase water concentration (C_{dw}) is calculated by using Equation 5-46. COPC-specific

bioaccumulation factor (BAF_{fish}) values are presented in Appendix A-3.

5.7.5.3 Fish Concentration (C_{fish}) from Biota-To-Sediment Accumulation Factors Using COPC Sorbed to Bed Sediment

U.S. EPA OSW recommends the use of Equation 5-50 to calculate fish concentration from *BSAF*s using

COPC sorbed to bed sediment for very hydrophobic compounds such as dioxins, furans, and PCBs. The

equation is also presented in Appendix B, Table B-4-28.

Recommended Equation for Calculating:
Fish Concentration (C_{fish}) from Biota-To-Sediment Accumulation Factors *(BSAF)*
Using COPC Sorbed to Bed Sediment

$$C_{fish} = \frac{C_{sb} \cdot f_{lipid} \cdot BSAF}{OC_{sed}}$$ Equation 5-50

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where

C_{fish}	=	Concentration of COPC in fish (mg COPC/kg FW tissue)
C_{sb}	=	Concentration of COPC sorbed to bed sediment (mg COPC/kg bed sediment)
f_{lipid}	=	Fish lipid content (unitless)
$BSAF$	=	Biota-to-sediment accumulation factor (unitless)
OC_{sed}	=	Fraction of organic carbon in bottom sediment (unitless)

The concentration of COPC sorbed to bed sediment (C_{sb}) is calculated by using Equation 5-47. U.S. EPA OSW recommended default values for the fish lipid content (f_{lipid}) and for the fraction of organic carbon in bottom sediment (OC_{sed}) are given in Appendix B, Table B-4-28. Biota-to-sediment accumulation factors ($BSAF$), which are applied only to dioxins, furans, and PCBs, are presented in Appendix A-3.

The use of Equation 5-50 to calculate fish concentration from bed sediment is consistent with U.S. EPA (1994r) and NC DEHNR (1997). Values recommended by U.S. EPA (1993h) range from 0.03 to 0.05 for the fraction of organic carbon in bottom sediment (Oc_{sed}). These values are based on an assumption of a surface soil OC content of 0.01. This document states that the organic carbon content in bottom sediments is higher than the organic carbon content in soils because (1) erosion favors lighter-textured soils with higher organic carbon contents, and (2) bottom sediments are partially comprised of detritus materials.

U.S. EPA (1993g) recommended a default value of 0.04 for OC_{sed}, which is the midpoint of the specified range. U.S. EPA (1993h; 1993g) recommended the use of 0.07 as the fish lipid content (f_{lipid}). This value was originally cited in Cook, Duehl, Walker, and Peterson (1991).

5.8   Use of Site-Specific vs. Default Parameter Values

As discussed in Chapter 1, most of the input parameters recommended for use in this guidance are not site-specific. After completing a risk assessment based on the default parameter values recommended in this guidance, risk assessors may choose to investigate the use of site-specific parameter values in order to provide a more representative estimate of site-specific risk. Use of parameter values other than those specified in this guidance should always be clearly described in the risk assessment report and work plan,

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and approved by the permitting authority. U.S. EPA OSW recommends that requests to change default

parameter values include the following information, as appropriate:

1.   An explanation of why the use of a more site-specific parameter value is warranted
        (e.g., the default parameter is based on data or studies at sites in the northwestern U.S.,
        but the facility is located in the southeast);

2.   The technical basis of the site-specific parameter value including readable copies of any
        relevant technical literature or studies;

3.   The basis of the default parameter value, as understood by the requestor, including
        readable copies of the referenced literature or studies (if available);

4.   A comparison of the weight-of-evidence between the competing studies (e.g., the
        site-specific parameter value is based on a study that is more representative of site
        conditions, a specific exposure setting being evaluated, or a more scientifically valid
        study than the default parameter, the site-specific parameter is based on the analysis of
        15 samples as opposed to 5 for the default parameter, or the site-specific study used more
        stringent quality control/quality assurance procedures than the study upon which the
        default parameter is based);

5.   A description of other risk assessments or projects where the site-specific parameter
        value has been used, and how such risk assessments or projects are similar to the risk
        assessment in consideration.

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